

DISCRETE SYMMETRY AND STABILITY IN HAMILTONIAN DYNAMICS

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In the present tutorial we address a problem with a long history, which remains of great interest to date due to its many important applications: It concerns the existence and stability of periodic and quasiperiodic orbits in N - degree of freedom Hamiltonian systems and their connection with discrete symmetries. Of primary importance in our study is what we call nonlinear normal modes (NNMs), i.e periodic solutions which represent continuations of the system's linear normal modes in the nonlinear regime. We examine questions concerning the existence of such solutions and discuss different methods for constructing them and studying their stability under fixed and periodic boundary conditions.

In the periodic case, we find it particularly useful to approach the problem through the discrete symmetries of many models, employing group theoretical concepts to identify a special type of NNMs which we call one-dimensional "bushes". We then describe how to use linear combinations of $s \geq 2$ such NNMs to construct s -dimensional bushes of quasiperiodic orbits, for a wide variety of Hamiltonian systems including particle chains, a square molecule and octahedral crystals in 1,2 and 3 dimensions. Next, we exploit the symmetries of the linearized equations of motion about these bushes to demonstrate how they may be simplified to study the destabilization of these orbits, as a result of their interaction with NNMs not belonging to the same bush. Applying this theory to the famous Fermi Pasta Ulam (FPU) chain, we review a number of interesting results concerning the stability of NNMs and higher-dimensional bushes, which have appeared in the recent literature.

We then turn to a newly developed approach to the analytical and numerical construction of quasiperiodic orbits, which does not depend on the symmetries or boundary conditions of our system. Using this approach, we demonstrate that the well-known "paradox" of FPU recurrences may in fact be explained in terms of the *exponential localization* of the energies E_q of NNM's being excited at the low part of the frequency spectrum, i.e. $q = 1, 2, 3, \dots$. These results indicate that it is the stability of these low-dimensional compact manifolds called q -tori, that is related to the persistence or FPU recurrences at low energies. Finally, we discuss a novel approach to the stability of orbits of conservative systems, expressed by a spectrum of indices called $GALI_k$,

$k = 2, \dots, 2N$, by means of which one can determine accurately and efficiently the destabilization of q tori, leading, after very long times, to the breakdown of recurrences and, ultimately, to the equipartition of energy, at high enough values of the total energy E .

Keywords: discrete symmetries; Hamiltonian systems; nonlinear normal modes; periodic and quasiperiodic orbits; stability; chaos

1. Introduction

The dynamics of Hamiltonian systems, or, more generally, conservative mechanical systems (preserving phase space volume) is of great importance for the understanding of many problems arising in classical mechanics, astronomy, solid state physics, plasma physics and nonlinear optics. The simplest states of such systems are their equilibrium points, where all variables are fixed for all time, and their periodic orbits, where all particles oscillate and return to their starting values after a time interval T . The first question concerning these states is their *existence*. Once this has been established, what one needs to know is their *stability*, i.e. their behavior under small perturbations of the initial conditions and parameter values. Two great contemporary scientists were the first to deal with these issues in a systematic and comprehensive way: The Russian mathematician Alexander Mikhailovich Lyapunov (1857 - 1918) and the French mathematical physicist Henri Poincaré (1854 - 1917). Lyapunov devoted a great deal of his efforts to ‘local’ stability analysis, obtaining specific conditions for the behavior of solutions of systems of ordinary differential equations (ODEs) in the vicinity of equilibrium points [Lyapunov, 1892]. Poincaré was more concerned with ‘global’ properties of the dynamics, like non - integrability and the occurrence of irregular (or chaotic) solutions, wandering over large domains of the available state space [Poincaré, 1892]. Remarkably, both of them worked on periodic solutions of N - degree - of - freedom Hamiltonian systems and were fascinated by the problem of the stability of the solar system.

In the present paper, our purpose is to review certain recent results concerning the dynamics of Hamiltonian systems of N degrees of freedom, whose equations of motion have the form

$$\frac{dq_k}{dt} = \frac{\partial H}{\partial p_k}, \quad \frac{dp_k}{dt} = -\frac{\partial H}{\partial q_k}, \quad k = 1, 2, \dots, N \quad (1)$$

In many cases the Hamiltonian is expanded in power series in the variables of positions and momenta, as a sum of homogeneous polynomials H_m of degree $m \geq 2$

$$H = H_2 + H_3 + \dots + H_m = E, \quad H_m = H_m(q_1, \dots, q_N, p_1, \dots, p_N) \quad (2)$$

(E is the total constant energy), so that the origin, $q_k = p_k = 0$, $k = 1, 2, \dots, N$ is an equilibrium point of the system. However, there also many examples, e.g. possessing discrete symmetries, for which no such decomposition is necessary as one can work directly with the original Hamiltonian.

Assume now that the linear equations resulting from (1) and (2) with $H_m = 0$, for all $m > 2$, yield a matrix, whose eigenvalues all occur in conjugate imaginary pairs, $\pm i\lambda_k$ and provide the frequencies of the so-called normal mode oscillations of the linearized system. According to Lyapunov, if *none* of the ratios of these eigenvalues, λ_j/λ_k , is an integer, for any $j, k = 1, 2, \dots, N$, the linear normal modes continue to exist as periodic solutions of the nonlinear system (1), when higher order terms H_3, H_4, \dots etc. are taken into account in (2). These solutions have frequencies close to those of the linear modes and are examples of what we call *nonlinear normal modes* (NNMs), where all variables (q_k, p_k) oscillate with the same frequency ($\lambda_j = \omega_j = 2\pi/T_j$, returning to the same values after a single maximum (and minimum) in their time evolution over one period T_j).

What is the importance of these periodic solutions? Once we have determined that they exist, what can we say about their stability properties under small perturbations? How do these change when we vary the total energy E in (2)? Does their loss of stability affect only their immediate vicinity or can they also influence the dynamics of the system as a whole? These are the questions we shall try to answer in this paper.

Let us consider, as a specific example, a mechanical system in one dimension described by the the N -particle Hamiltonian

$$H = \frac{1}{2} \sum_{k=1}^N p_k^2 + \frac{1}{2} \sum_{k=0}^N (x_{k+1} - x_k)^2 + \frac{\alpha}{3} \sum_{k=0}^N (x_{k+1} - x_k)^3 + \frac{\beta}{4} \sum_{k=0}^N (x_{k+1} - x_k)^4 = E \quad (3)$$

called the FPU chain in honor of Fermi, Pasta and Ulam, who were the first to study it numerically in the early 1950's [Fermi *et al.*, 1955]. They discovered certain very interesting and surprising phenomena concerning its dynamics, which we will discuss later in this review. For the time being, let us note that when this chain is studied under *fixed* boundary conditions (f.b.c.), i.e. $x_0 = x_{N+1} = 0$, there are many N 's for which the linear normal mode frequencies satisfy the incommensurability condition of Lyapunov's theorem and hence they may be rigorously continued to the nonlinear regime of $\alpha \neq 0$ and/or $\beta \neq 0$.

By contrast, when *periodic* boundary conditions (p.b.c.) are imposed, i.e. $x_j = x_{j+N}$, $p_j = p_{N+j}$, $j = 1, 2, \dots, N$, the linear mode spectrum becomes degenerate for *all* N and Lyapunov's theorem cannot be invoked. What do we do in that case? How do we study the existence and stability of such nonlinear normal modes, or NNMs? As we explain at length in sections II and III, this is an important case where the identification and analysis of the system's *discrete symmetries* turns out to be of great relevance to the understanding of the dynamics of the problem.

Thus, we start by demonstrating in section II precisely how one can use the powerful techniques of group theory to establish the existence of families of such NNMs for a variety of mechanical systems, including particle chains in one dimension (under p.b.c.), as well as certain 2-dimensional and 3-dimensional structures. Then, in section III, we show how one can combine such periodic solutions to form "bushes" of quasiperiodic orbits and exploit the symmetries of the system to simplify the variational equations about these orbits and study the motion in their vicinity. Ultimately, of course, one would like to be able to obtain *invariant manifolds* on which the dynamics of the system is as simple as possible. This is not easy to do in general, but if the equations of motion possess discrete symmetry groups, one can single out some of these manifolds using regular group theoretical methods developed in [Sakhnenko & Chechin, 1993, 1994; Chechin & Sakhnenko, 1998]. These methods provide, in fact, the mathematical basis of the theory of *bushes* of NNMs, which plays an important role in many of the results discussed in this review.

Before discussing this theory, however, let us illustrate its main ingredients on a seemingly simple example of an N degree of freedom Hamiltonian system. In particular, let us consider the famous Fermi-Pasta-Ulam β -chain (FPU- β), i.e. Eq. (99) with $\alpha = 0$, representing a one-dimensional lattice of unit masses coupled to each other by identical nonlinear springs (see Fig. 1). The ordinary differential equations (ODEs)

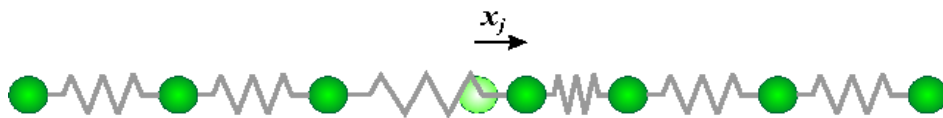


Fig. 1. FPU chain.

describing longitudinal vibrations of the FPU- β chain can be written in the form

$$\ddot{x}_i = f(x_{i+1} - x_i) - f(x_i - x_{i-1}), \quad i = 1..N, \quad (4)$$

where $x_i(t)$ is the displacement of the i th particle from its equilibrium state at time t , while the force $f(\Delta x)$ depends on the spring deformation Δx as

$$f(\Delta x) = \Delta x + \beta(\Delta x)^3 \quad (5)$$

For simplicity, we assume that $\beta > 0$, since in that case the potential is positive definite everywhere and particles cannot escape to infinity. If we also impose p.b.c. we must require:

$$x_{N+1}(t) \equiv x_1(t), \quad x_0(t) \equiv x_N(t). \quad (6)$$

Thus, we shall study possible dynamical regimes of this chain by attempting to solve (4) for the “configuration” vector

$$\vec{X}(t) = \{x_1(t), x_2(t), \dots, x_N(t)\} \quad (7)$$

whose components are the individual particle displacements.

As is well-known, it is pointless to try to obtain this vector as a general solution of (4). We will, therefore, concentrate on studying special solutions represented by the NNMs mentioned above. In particular, let us begin with the following simple periodic solution

$$\vec{X}(t) = \{x(t), -x(t), x(t), -x(t), \dots, x(t), -x(t)\} \quad (8)$$

which is easily seen to exist in the FPU chain with an even number of particles ($N \bmod 2 = 0$). This solution is fully determined by *only one* arbitrary function $x(t)$ and is called “ π -mode” or boundary zone mode.

From Eq. (8), it is evident that every two neighboring particles possess equal in value but opposite in sign displacements at any instant t . To investigate the dynamical regime of this mode in the FRU- β chain, let us substitute $\vec{X}(t)$ from Eq. (8) in Eq. (4), taking into account Eqs. (5) and (6). As a result, all N equations (4) become *identical* and can be written in the form:

$$\ddot{x} + \omega^2 x + \gamma \left(\frac{\beta}{N} \right) x^3 = 0, \quad (9)$$

where $\omega^2 = 4$, $\gamma = 16$ and the x_i have been scaled by a factor $1/\sqrt{N}$.

This is the well-known Duffing’s equation. In the case $\beta > 0$ it describes periodic vibrations with arbitrary fixed amplitude A determined by initial conditions which have the form

$$x(0) = A, \quad \dot{x}(0) = 0. \quad (10)$$

As is well-known, the analytical solution to Eqs. (9), (10) can be expressed via the Jacobi elliptic cosine [Abramowitz & Stegun, 1965]:

$$x(t) = A \operatorname{cn}(\Omega t, k^2), \quad (11)$$

where

$$\Omega^2 = \omega^2 / (1 - 2k^2), \quad (12)$$

while the modulus k of this elliptic function is determined by the relations

$$2k^2 = \frac{bA^2}{\omega^2 + bA^2}, \quad b = \gamma \left(\frac{\beta}{N} \right). \quad (13)$$

Thus, the so-called π -mode defined by Eq. (8) describes an *exact* dynamical regime of the nonlinear system. It represents an example of the type of nonlinear normal modes introduced by Rosenberg [Rosenberg, 1962]. From Eqs. (11, 13) it can be seen that in the low-amplitude limit ($A \rightarrow 0$) the above NNM is an exact continuation of the *linear normal mode* ($k \rightarrow 0$, $\Omega \rightarrow \omega$), as the elliptic cosine tends to the ordinary cosine.

NNMs exist in Hamiltonian systems with rather specific interparticle interactions, as, for example, in cases where the potential energy is a *homogeneous* function of all its arguments. In many cases, however, the existence of NNMs may be established by certain symmetry related arguments, whence we refer to such dynamical objects as *symmetry-determined* NNMs.

The π -mode (8) clearly represents a dynamical state of the form:

$$\vec{X}(t) = x(t)\{1, -1, |1, -1, \dots, |1, -1\}. \quad (14)$$

Hence, the following question naturally arises: Are there any other such exact NNMs in the FPU- β chain, under p.b.c.? Some examples of such modes are already known in the literature [Poggi & Ruffo, 1997; Rink, 2003; Shinohara, 2002, 2003; Yoshimura, 2004; Leo & Leo, 2007; Antonopoulos & Bountis, 2006; Kosevich, 1993], under a terminology that differs among authors. Below we list these exact states in detail:

$$\vec{X}(t) = x(t)\{1, 0, -1, |1, 0, -1, |, \dots, |1, 0, -1\}, \quad \omega^2 = 3, \quad \gamma = \frac{27}{2} \quad (N \bmod 3 = 0). \quad (15)$$

$$\vec{X}(t) = x(t)\{1, -2, 1, |1, -2, 1, |, \dots, |1, -2, 1\}, \quad \omega^2 = 3, \quad \gamma = \frac{27}{2} \quad (N \bmod 3 = 0). \quad (16)$$

$$\vec{X}(t) = x(t)\{0, 1, 0, -1, |0, 1, 0, -1, |, \dots, |0, 1, 0, -1\}, \quad \omega^2 = 2, \quad \gamma = 4 \quad (N \bmod 4 = 0). \quad (17)$$

$$\begin{aligned} \vec{X}(t) &= x(t)\{1, 1, -1, -1|1, 1, -1, -1|, \dots, |1, 1, -1, -1\}, \\ \omega^2 &= 2, \quad \gamma = 8 \quad (N \bmod 4 = 0). \end{aligned} \quad (18)$$

$$\begin{aligned} \vec{X}(t) &= x(t)\{0, 1, 1, 0, -1, -1|0, 1, 1, 0, -1, -1|, \dots, |0, 1, 1, 0, -1, -1\}, \\ \omega^2 &= 1, \quad \gamma = \frac{3}{2} \quad (N \bmod 6 = 0). \end{aligned} \quad (19)$$

Let us comment on certain properties of the above NNMs for the FPU- β chain, having an appropriate number of particles in every case:

P1) *Displacement patterns* of NNMs (14) - (19) are defined in terms of the vibrational state primitive cells (divided by vertical lines), whose number of elements m is called the multiplicity number.

For (14) - (19) these numbers have the values: $m = 2$ for Eq. (14), $m = 3$ for Eqs. (15) and (16), $m = 4$ for Eqs. (17) and (18) and $m = 6$, for Eq. (19). Note that, due to p.b.c., the FPU- β chain in its *equilibrium* state is invariant under translation by the interparticle distance a , while in its *vibrational* states it is invariant under a translation by ma . Moreover, NNMs (14) - (19) do not differ only by translational symmetry (ma), but also by some additional symmetry transformations which are discussed later in this paper.

P2) Each of the NNMs (14) - (19) depends on *only one* function $x(t)$ and, therefore, describes a single *one-dimensional* dynamical regime. This function satisfies Duffing's equation (9), with ω^2 and γ that differ according to the displacement pattern of each NNM.

P3) Every NNM (15) - (19) possesses some "dynamical domain" of its own. For example, consider the mode (15): It is easy to check that cyclic permutations of each primitive cell in its displacement pattern produces *other* modes: $x(t)\{1, 0, -1, |1, 0, -1, |, \dots, |1, 0, -1\} \rightarrow x(t)\{0, -1, 1, |0, -1, 1, |, \dots, |0, -1, 1, \} \rightarrow x(t)\{-1, 1, 0, |-1, 1, 0, |, \dots, |-1, 1, 0, \}$, which differ from each other only by the position of their *stationary* particles.

As a consequence, all dynamical properties of these NNMs turn out to be *equivalent*. In particular, as we shall show in detail in section III, they possess the same stability regions. Because of this reason, we only need to study one representative of the set of equivalent NNMs. Such sets are called "dynamical domains", borrowing the term from the theory of phase transitions in crystals.

Many aspects of existence and stability of NNMs have been discussed in the literature (see, for example, [Chechin *et al.*, 2002, 2005; Rink, 2003; Poggi & Ruffo, 1997; Shinohara, 2002, 2003; Yoshimura, 2004; Leo & Leo, 2007; Antonopoulos & Bountis, 2006; Budinsky & Bountis, 1983; Sandusky & Page, 1994; Kosevich, 1993]). What is important at this point is to pose certain fundamental questions concerning such NNMs, which we shall proceed to answer in this review to the best of our ability:

Q1) Is the list (14) - (19) of NNMs for the FPU- β chain complete?

Indeed, at first sight, it seems that many other NNMs can exist, for example, modes whose multiplicity number m is different from those listed above.

Q2) What kind of NNMs exist in nonlinear chains with different interactions than those of the FPU- β chain?

In fact, in most papers (see [Poggi & Ruffo, 1997; Shinohara, 2002, 2003; Yoshimura, 2004; Kosevich, 1993]) the NNMs listed as (14) - (19) above have been discussed by analyzing dynamical equations which are only connected with the FPU- β interparticle interaction.

Q3) Do there exist NNMs for Hamiltonian systems which are more complicated than the monoatomic chains? For example, one can pose this question for diatomic nonlinear chains (with particles having alternating masses), 2-dimensional (2D) lattices, or 3D crystal structures.

Q4) Finally, there is a more subtle issue: How can one construct exact *multidimensional* dynamical regimes in nonlinear N -particle Hamiltonian systems and study their stability by locating the unstable manifolds of the corresponding quasiperiodic orbits?

Note that the NNMs discussed so far represent exact *one-dimensional* regimes, because they are fully determined by only one time-dependent function. As we shall discover in subsequent sections, there exist very interesting dynamical regimes of regular motion depending on more than one frequency and characterized by families of quasiperiodic functions, forming s -dimensional tori, with $s \geq 2$.

Such exact regimes of nonlinear mechanical systems, identified by discrete symmetry, are called *bushes* of NNMs. For example, the following two-dimensional bush exists in the FPU- β chain with $N \bmod 6 = 0$:

$$\vec{X}(t) = \{0, x_1(t), x_2(t), 0, -x_2(t), -x_1(t) | \dots | 0, x_1(t), x_2(t), 0, -x_2(t), -x_1(t)\} \quad (20)$$

This bush, with multiplicity number $m = 6$, is determined by two functions, $x_1(t)$ and $x_2(t)$, satisfying a system of two nonlinear autonomous ODEs.

In contrast to *one-dimensional* bushes, *multidimensional* bushes also exist, representing exact *quasiperiodic* dynamical regimes. In the framework of the bush theory, the problem of finding exact nonlinear regimes in a physical system with discrete symmetry can be solved *without* any information about interparticle interactions. However, the explicit form of the bush dynamical equations essentially depends on the interparticle interactions in the considered system.

Actually, the concept of bushes of NNMs and the group theoretical methods used for their construction constitute an extension of the theory of complete condensates developed in the papers [Chechin *et al.*, 1993, 1989; Chechin, 1989] studying phase transitions in solids. Note that the concept of bushes of NNMs does not apply only to vibrations of mechanical systems, since one may consider bushes of *any other physical nature*, for example, bushes of spin modes.

Thus, in sections II, III of this review, we attempt to show that the theory of bushes gives definite and quite general answers to the above questions Q1–Q3 in nonlinear systems with discrete symmetries. We then proceed to answer question Q4, using the recent analytical and numerical results described in section III.

More specifically, we demonstrate that it is possible to use Poincaré-Linstedt series expansions to construct exact quasiperiodic solutions with $s \geq 2$ frequencies, which belong to the lower part of the linear normal mode spectrum, with $q = 1, 2, 3, \dots$. We are thus able to establish the important property that the energies E_q excited by these low-dimensional, so-called q -tori, are exponentially localized in q -space [Christodoulidi *et al.*, 2010]. The relevance of this fact becomes apparent when we study the well-known phenomenon of FPU recurrences, which are remarkably persistent in FPU chains (with fixed or periodic boundary conditions), at low values of the total energy E .

We also study the stability of these q -tori as accurately as possible, using methods that do not rely on Floquet theory and are quite different than those adopted in section III. In particular, we make use of the novel method of the GALI_k indicators, $k = 2, \dots, 2N$, which distinguish rapidly and efficiently between chaotic and quasiperiodic orbits [Skokos *et al.*, 2007, 2008]. As predicted theoretically and verified extensively by numerical evidence, in the chaotic case all the GALIs decay exponentially, while in the quasiperiodic the first $s - 1$ GALIs are nearly constant (indicating the dimension s of the associated torus), while all others go to zero by power laws. Thus, by marking the total energy E at which the GALI_k , with the highest k , start to decrease exponentially, it is possible to determine the destabilization threshold at which the q -tori are destroyed, implying the breakdown of FPU recurrences and the eventual equipartition of energy among all modes.

2. Bushes of NNMs in configuration space

The theory of bushes of nonlinear normal modes was originally developed in [Sakhnenko & Chechin, 1993, 1994; Chechin & Sakhnenko, 1998], while its detailed description can be found in [Chechin *et al.*, 2007]. Low-dimensional bushes in mechanical systems with various kinds of symmetry and structures were studied in [Sakhnenko & Chechin, 1993, 1994; Chechin & Sakhnenko, 1998; Chechin *et al.*, 2007, 2003, 2002]. In particular, all possible symmetry-determined NNMs, representing one-dimensional bushes, for all N -particle mechanical systems with any of 230 *space groups* were found in [Chechin *et al.*, 2007].

The important problem of bush *stability* was discussed in [Chechin *et al.*, 2003, 2002, 2005], the first two of these papers being devoted to the vibrational bushes in Fermi-Pasta-Ulam chains. Some

theorems about bush structures and the *normal forms* of their dynamical equations were presented in [Chechin & Sakhnenko, 1998]. The general group theoretical method for the simplification of the bush stability analysis was presented in [Chechin & Zhukov, 2006].

Note that dynamical objects equivalent to the bushes of NNMs have also been discussed for *monoatomic chains* by several other authors [Rink, 2003; Poggi & Ruffo, 1997]. Let us emphasize, however, that the group theoretical methods developed in [Sakhnenko & Chechin, 1993, 1994; Chechin & Sakhnenko, 1998; Chechin & Zhukov, 2006] can be applied equally well not only to monoatomic chains (as illustrated in [Chechin *et al.*, 2002, 2005; Chechin & Zhukov, 2006]), but also to *any* other physical system with discrete symmetry groups (see [Chechin *et al.*, 2007]).

In this section, we shall demonstrate the power of bush theory methods using three simple mechanical models: A nonlinear chain of particles moving in one-dimension under p.b.c., a "square molecule" whose particles move in a two-dimensional plane and an octahedral structure of particles moving in three dimensions. For these nonlinear dynamical systems, we will consider different *vibrational* regimes and thus deal with bushes of *vibrational* modes.

Now, in order to properly define bushes of NNMs, one must first determine the *parent* symmetry group of the equations describing the vibrations of a given mechanical system.

2.1. Parent symmetry group

A parent symmetry group consists of all transformations which leave the system of dynamical equations *invariant*. In general, such transformations can include space and time variables as well as parameters of the system. Let us consider, for example, the dynamical equations (4) for the FPU- β chain with p.b.c. (6) and an even number of particles. It is easy to guess some space transformations which do not change Eqs. (4, 6) by considering the *equilibrium state* of our nonlinear chain. Firstly, this chain is invariant under the action of the operator \hat{a} which shifts it by the lattice spacing a . This operator generates the translational group

$$T = \{\hat{e}, \hat{a}, \hat{a}^2, \dots, \hat{a}^{N-1}\}, \quad \hat{a}^N = \hat{e}, \quad (21)$$

where \hat{e} is the identity element and N is the order of the cyclic group T . The operator \hat{a} induces the cyclic permutation of all particles of the chain and, therefore, acts on the configuration vector $\vec{X}(t)$ as follows:

$$\hat{a}\vec{X}(t) \equiv \hat{a}\{x_1(t), x_2(t), \dots, x_{N-1}(t), x_N(t)\} = \{x_N(t), x_1(t), x_2(t), \dots, x_{N-1}(t)\}. \quad (22)$$

Secondly, the symmetry group of the monoatomic chain contains the *inversion* \hat{i} , with respect to the center of the chain, which acts on the vector $\vec{X}(t)$ in the following way:

$$\begin{aligned} \hat{i}\vec{X}(t) &\equiv \hat{i}\{x_1(t), x_2(t), \dots, x_{N-1}(t), x_N(t)\} = \\ &= \{-x_N(t), -x_{N-1}(t), \dots, -x_2(t), -x_1(t)\}. \end{aligned} \quad (23)$$

The complete set of symmetry transformations includes also all products $\hat{a}^k \hat{i}$ of the pure translations \hat{a}^k ($k = 1, 2, \dots, N-1$) with the inversion \hat{i} and forms the so-called dihedral group D which can be written as a direct sum of the two *cosets* T and $T \cdot \hat{i}$:

$$D = T \oplus T \cdot \hat{i}. \quad (24)$$

This is a non-Abelian group induced by two *generators* (\hat{a} and \hat{i}) with the following *generating relations*

$$\hat{a}^N = \hat{e}, \quad \hat{i}^2 = \hat{e}, \quad \hat{i}\hat{a} = \hat{a}^{-1}\hat{i}. \quad (25)$$

When applied to Eqs. (4), operators \hat{a} and \hat{i} induce the following changes of variables:

$$\begin{aligned} \hat{a} : & x_1(t) \rightarrow x_2(t), x_2(t) \rightarrow x_3(t), \dots, x_{N-1}(t) \rightarrow x_N(t), x_N(t) \rightarrow x_1(t); \\ \hat{i} : & x_1(t) \leftrightarrow -x_N(t), x_2(t) \leftrightarrow -x_{N-1}(t), x_3(t) \leftrightarrow -x_{N-2}(t), \dots \end{aligned} \quad (26)$$

It is straightforward to check that upon acting on (4) with transformation (26) the system is transformed to an *equivalent* form. Moreover, since Eqs. (4) are invariant under the actions of \hat{a} and \hat{i} , they are also invariant with respect to all products of these two operators and, therefore, the dihedral group D is indeed a symmetry group of equations (4) for a monoatomic chain with *arbitrary* interparticle interactions.

As a consequence, the dihedral group D can be considered as a parent symmetry group for *all* monoatomic nonlinear chains as, for example, the FPU- α chain, whose interparticle interactions are characterized by the force

$$f(\Delta x) = \Delta x + \alpha(\Delta x)^2. \quad (27)$$

Of course, since in the case of the FPU- β chain the force $f(\Delta x) = \Delta x + \beta(\Delta x)^3$ is an *odd* function of its argument Δx , the FPU- β chain possesses a *higher* symmetry group than the FPU- α chain.

Indeed, let us introduce the operator \hat{u} which changes the signs of all atomic displacements without their transposition:

$$\hat{u}\vec{X} \equiv \hat{u}\{x_1(t), x_2(t), \dots, x_{N-1}(t), x_N(t)\} = \{-x_1(t), -x_2(t), \dots, -x_{N-1}(t), -x_N(t)\}. \quad (28)$$

It can easily be checked that the operator \hat{u} generates a transformation of all the variables $x_i(t)$, $i = 1..N$ in Eqs. (4)–(6), which leads to an equivalent form of these equations. Therefore, the operator \hat{u} and all its products with elements of the dihedral group D belong to the full symmetry group of the FPU- β chain.

Clearly, the operator \hat{u} *commutes* with all the elements of the dihedral group D and we can consider the group

$$G = D \oplus D \cdot \hat{u} \quad (29)$$

as the parent symmetry group of the FPU- β chain. The group G contains *twice as many* elements as the dihedral group D and, therefore, possesses a greater number of subgroups.

On the other hand, every subgroup of the parent group generates a certain bush of NNMs. Therefore, there exists a greater number of bushes for the FPU- β chain (and for any other chain with *odd* force of interparticle interactions) compared with those of the FPU- α chain (and for all arbitrary nonlinear monoatomic chains, as well).

Finally, let us note that it is sufficient for our purposes to define any symmetry group by listing only its *generators* which we denote by square brackets, for example, we write $T[\hat{a}]$, $D[\hat{a}, \hat{i}]$, $G[\hat{a}, \hat{i}, \hat{u}]$.

2.2. Subgroups of the parent group and bushes of NNMs

Let us consider now a specific configuration vector $\vec{X}^{(j)}(t)$ [see Eq. (7)], which determines a displacement pattern at time t , and let us act on it successively by the operators \hat{g} that correspond to all the elements of a parent group G_0 . The full set G_j of elements of the group G_0 , under which $\vec{X}^{(j)}(t)$ turns out to be *invariant*, generates a certain *subgroup* of the group G_0 ($G_j \subset G_0$) [Note that this subgroup can be *trivial*, i.e. it can consist of only one symmetry element \hat{e} . In this case, a chosen configuration vector $\vec{X}^{(j)}(t)$ turns out to be of general form, since there are no connections between the displacements of different particles of the chain]. We then call $\vec{X}^{(j)}(t)$ invariant under the action of the subgroup G_j of the parent group G_0 and use it to determine the bush of nonlinear normal modes corresponding to the subgroup G_j of the group G_0 .

Therefore, in the framework of the above approach, one must find all the subgroups of the parent group G_0 to obtain all the bushes of NNMs of different types,. This can be done by standard group theoretical methods. In [Chechin *et al.*, 2005] a simple crystallographic technique was developed for singling out all the subgroups of the parent group of any monoatomic chain, following the approach of a more general method [Chechin *et al.*, 1993, 1989; Chechin, 1989]. We shall not discuss here how to find subgroups of the parent groups; rather, we will demonstrate how one can obtain bushes of NNMs if the subgroups are already known.

Let us consider the subgroups G_j of the dihedral group D . Each group G_j contains its own *translational subgroup* $T_j \subset T$, where T is the above discussed full translational group (21). If N is divisible by 4 (for example, we consider below the case $N = 12$) there exists a subgroup $T_4 = [\hat{a}^4]$ of the group $T = [\hat{a}]$. Note that, in square brackets, we write down only the generators of the considered group, while the complete set of group elements is written in curly brackets, as, for example, in Eq. (21).

If a vibrational state of the chain possesses the symmetry group $T_4 = [\hat{a}^4] \equiv \{\hat{e}, \hat{a}^4, \hat{a}^8, \dots, \hat{a}^{N-4}\}$, the displacements of the atoms, which are at a distance $4a$ from each other in the equilibrium state, turn out

to be *equal*, since the operator \hat{a}^4 leaves the vector $\vec{X}(t)$ invariant. For example, for the case $N = 12$, the operator \hat{a}^4 permutes the coordinates of $\vec{X} = (x_1, x_2, \dots, x_{12})$ taken in quadruplets $(x_i, x_{i+1}, x_{i+2}, x_{i+3})$, $i = 1, 5, 9$, while from equation $\hat{a}^4 \vec{X}(t) = \vec{X}(t)$ one deduces $x_i = x_{i+4}$, $i = 1, 2, 3, 4$. Thus, the vector $\vec{X}(t)$ contains 3 times the quadruplets x_1, x_2, x_3, x_4 , where $x_i(t)$ ($i = 1, 2, 3, 4$) are arbitrary functions of time and can be written as follows

$$\vec{X}(t) = \{ x_1(t), x_2(t), x_3(t), x_4(t) \mid x_1(t), x_2(t), x_3(t), x_4(t) \mid x_1(t), x_2(t), x_3(t), x_4(t) \}. \quad (30)$$

In other words, the complete set of atomic displacements can be divided into $N/4$ (in our case, $N/4 = 3$) *identical* subsets, which are called “extended primitive cells” (EPC). In the bush (30), the EPC contains four atoms, and the vibrational state of the whole chain is described by three such EPC. Thus, the EPC for the vibrational state with the symmetry group $T_4 = [\hat{a}^4]$ has size equal to $4a$, which is four times larger than the primitive cell of the chain in the equilibrium state.

It is essential that some symmetry elements of the dihedral group D disappear as a result of the symmetry reduction $D = [\hat{a}, \hat{i}] \rightarrow T_4 = [\hat{a}^4]$. There are four other subgroups of the dihedral group D , corresponding to the same translational subgroup $T_4 = [\hat{a}^4]$:

$$[\hat{a}^4, \hat{i}], \quad [\hat{a}^4, \hat{a}\hat{i}], \quad [\hat{a}^4, \hat{a}^2\hat{i}], \quad [\hat{a}^4, \hat{a}^3\hat{i}]. \quad (31)$$

Each of these subgroups possesses *two generators*, namely \hat{a}^4 and an inversion element $\hat{a}^k\hat{i}$ ($k = 0, 1, 2, 3$). Note that the $\hat{a}^k\hat{i}$ differ from each other by the *position* of the center of inversion.

Subgroups $[\hat{a}^4, \hat{a}^k\hat{i}]$ with $k > 3$ are equivalent to those listed in (31), since the second generator $\hat{a}^k\hat{i}$ can be multiplied from the left by \hat{a}^{-4} , representing the inverse element with respect to the generator \hat{a}^4 . Thus, there exist only five subgroups of the dihedral group (with $N \bmod 4 = 0$) constructed on the basis of the translational group $T_4 = [\hat{a}^4]$, namely, this group and the four groups from the list (31).

Now, let us examine the bushes corresponding to the subgroups (31). The subgroup $[\hat{a}^4, \hat{i}]$ consists of the following six elements:

$$\hat{e}, \hat{a}^4, \hat{a}^8, \hat{i}, \hat{a}^4\hat{i}, \hat{a}^8\hat{i} \equiv \hat{i}\hat{a}^4. \quad (32)$$

The invariance of $\vec{X}(t)$ with respect to this group can be written as follows:

$$\hat{a}^4 \vec{X}(t) = \vec{X}(t), \quad \hat{i} \vec{X}(t) = \vec{X}(t), \quad (33)$$

while the invariance of the vector $\vec{X}(t)$ under the action of the group generators $[\hat{a}^4$ and $\hat{i}]$ guarantees its invariance under all elements of this group.

As explained above, the equation $\hat{a}^4 \vec{X}(t) = \vec{X}(t)$ is satisfied by the vector $\vec{X}(t)$, see (30), while $\hat{i} \vec{X}(t) = \vec{X}(t)$ also holds, from which we obtain the following relations for each of the three EPS: $x_1(t) = -x_4(t)$, $x_2(t) = -x_3(t)$.

Therefore, for $N = 12$, the invariant vector $\vec{X}(t)$ of the group $[\hat{a}^4, \hat{i}]$ can be written in the form

$$\vec{X}(t) = \{x_1(t), x_2(t), -x_2(t), -x_1(t) \mid x_1(t), x_2(t), -x_2(t), -x_1(t) \mid x_1(t), x_2(t), -x_2(t), -x_1(t)\}, \quad (34)$$

where $x_1(t)$ and $x_2(t)$ are arbitrary functions of time.

Thus, the subgroup $[\hat{a}^4, \hat{i}]$ of the dihedral group D generates a *two-dimensional* bush of NNMs. The explicit form of the differential equations governing the two variables $x_1(t)$ and $x_2(t)$ can now be obtained by substitution of the ansatz (34) into the FPU- β dynamical equations (4-6). We shall, hereafter, denote the bush (34) in the form

$$B[\hat{a}^4, \hat{i}] = |x_1, x_2, -x_2, -x_1|, \quad (35)$$

showing the atomic displacements *in only one EPS* and omitting the argument t of variables $x_1(t)$, $x_2(t)$.

Proceeding in a similar manner, we obtain bushes of NNMs for three other groups from the list (31):

$$B[\hat{a}^4, \hat{a}\hat{i}] = |0, x, 0, -x|, \quad (36)$$

$$B[\hat{a}^4, \hat{a}^2\hat{i}] = |x_1, -x_1, x_2, -x_2|, \quad (37)$$

$$B[\hat{a}^4, \hat{a}^3 \hat{i}] = |x, 0, -x, 0|, \quad (38)$$

Let us comment on these results: The bushes $B[\hat{a}^4, \hat{a} \hat{i}]$ and $B[\hat{a}^4, \hat{a}^3 \hat{i}]$ turn out to be one-dimensional in the sense that they represent simple periodic solutions corresponding to NNMs. These modes are, in fact, *equivalent* since they differ from each other only by the numbering of the particles on the chain. In group theoretical terms, this equivalence is a consequence of the fact that $G_1 = [\hat{a}^4, \hat{a} \hat{i}]$ and $G_2 = [\hat{a}^4, \hat{a}^3 \hat{i}]$ prove to be conjugate¹ subgroups in the parent group $D = [\hat{a}, \hat{i}]$. Both two-dimensional bushes (35) and (37) are also equivalent to each other for the same reason.

All displacement patterns (35-38) are particular cases of the general pattern of the bush $B[\hat{a}^4] = |x_1, x_2, x_3, x_4|$. One may, therefore, ask what will happen during time evolution of *other* particular cases of $B[\hat{a}^4]$. For example, if one chooses for the FPU β -chain with $N \bmod 4 = 0$ an initial one-dimensional pattern of the form $\vec{X}(0) = \{3x_0, -x_0, -x_0 | 3x_0, -x_0, -x_0 | \dots\}$ or, for $N \bmod 5 = 0$, an initial state of the type $\vec{X}(0) = \{-x_0, -x_0, 4x_0, -x_0, -x_0 | -x_0, -x_0, 4x_0, -x_0, -x_0 | \dots\}$ one easily finds that there are *no subgroups* of the parent group D which produce these displacement patterns. As a consequence, when solving the equations of motion of the FPU- β chain in these cases to obtain $\vec{X}(t)$, the above structures will *not be conserved* in time.

More generally, we conclude that for *sufficiently large* EPS there are not enough symmetry elements to give rise to NNMs, since the bushes of the corresponding displacement patterns are multidimensional. For this reason, there exists only a very specific number of bushes for any fixed dimension beyond the NNMs!

2.3. Bushes of NNMs for arbitrary interparticle interactions

As was proved in [Chechin *et al.*, 2005] for any nonlinear monoatomic chain with *arbitrary* interparticle interactions, there exist *only three* symmetry-determined NNMs:

$$B[\hat{a}^2, \hat{i}] = |x, -x|, (\pi\text{-mode}), \quad B[\hat{a}^3, \hat{i}] = |x, 0, -x|, \quad B[\hat{a}^4, \hat{a} \hat{i}] = |0, x, 0, -x|. \quad (39)$$

(each NNM corresponds to a certain subgroup of the *dihedral* group D). These modes can easily be excited in the FPU- α and FPU- β chains, if we solve numerically the corresponding dynamical equations with appropriate initial conditions.

On the other hand, it is already known that the FPU- β chain possesses a *higher* symmetry group G , since changing signs of all the displacements by the operator \hat{u} [see Eq. (28)] leaves the FPU- β dynamical equations invariant. Therefore, all subgroups of the group D also turn out to be subgroups of the group G , while G possesses some *additional* subgroups whose elements can contain the operator \hat{u} .

As a consequence, there exist more bushes of NNMs for the FPU- β chain (and for any other chain with *odd* force of interparticle interactions) than for the FPU- α chain (or any other chain whose interparticle interactions is not described by odd function $f(\Delta x)$). These additional bushes were presented in [Chechin *et al.*, 2005] in the following form:

$$B[\hat{a}^3, \hat{i} \hat{u}] = |x, -2x, x|, \quad B[\hat{a}^2 \hat{u}, \hat{i}] = |x, x, -x, -x|, \quad B[\hat{a}^3 \hat{u}, \hat{a} \hat{i}] = |0, x, x, 0, -x, -x|. \quad (40)$$

and were also obtained in [Rink, 2003] by a different method.

2.4. Bushes of NNMs for a square molecule

In our model, a square molecule is represented by a mechanical system whose equilibrium state is depicted in Fig. 2. Four atoms of this molecule are shown as filled circles at the vertices of the square. The number of every atom and its (x, y) coordinates are as given in the figure.

Let us suppose that atoms can oscillate about their equilibrium positions only in the (x, y) plane and, therefore, eight degrees of freedom are needed to describe this mechanical system. Furthermore, we will

¹Two subgroups G_1 and G_2 of the same group G are called conjugate to each other, if there exists at least one element $g_0 \in G$ which converts G_1 into G_2 via the transformation $G_2 = g_0^{-1} G_1 g_0$. [note that in the case of bushes (36) and (38), $g_0 = \hat{a}$].

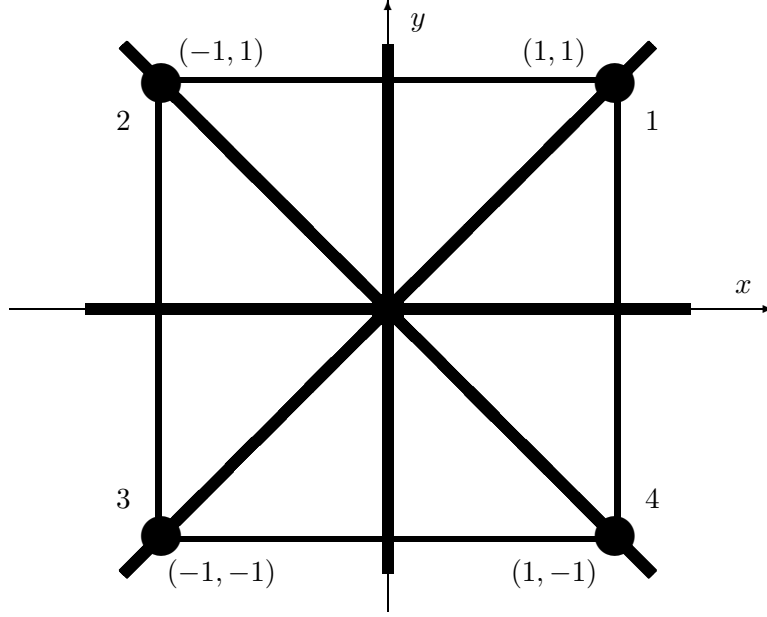


Fig. 2. Mechanical model of a square molecule.

not consider any specific type of interparticle interactions and treat bushes of NNMs as purely geometrical objects. The equilibrium configurations of our molecule possess the symmetry group denoted by C_{4v} in the Schoenflies notation, while, at equilibrium, the molecule depicted in Fig. 2 is invariant under the action of the following transformations:

- Rotations through the angles 0° , 90° , 180° , 270° about the z axis orthogonal to the plane of Fig. 2 and passing through the center of the square. We will denote these rotations by g_1 , g_2 , g_3 , g_4 , respectively.
- Reflections in four mirror planes orthogonal to the plane of Fig. 2 and passing through the z axis. (We depict these mirror planes by bold lines). Two of them are “coordinate” planes (g_5 , g_7) and the other two are “diagonal” planes (g_6 , g_8).

Analytically, the above mentioned symmetry elements can be defined as follows:

$$\begin{aligned} g_1(x, y) &= (x, y), & g_2(x, y) &= (-y, x), & g_3(x, y) &= (-x, -y), & g_4(x, y) &= (y, -x) \\ g_5(x, y) &= (-x, y), & g_6(x, y) &= (-y, -x), & g_7(x, y) &= (x, -y), & g_8(x, y) &= (y, x) \end{aligned} \quad (41)$$

Thus, the symmetry group of the square molecule (C_{4v}) contains 8 elements g_1, \dots, g_8 , determined by Eq. (41). This group is non-Abelian since, for example, $g_2 \cdot g_8 = g_5$, while $g_8 \cdot g_2 = g_7$. According to Lagrange’s theorem, the order of any subgroup is a *divisor* of the order of the full group. Therefore, for the case of the group $G = C_{4v}$ with the order $m = \|G\| = 8$, there exist only subgroups G_j with order equal to $m = 1, 2, 4, 8$ given by the following list:

$$\begin{aligned} m = 1 : & G_1 = \{g_1\} = C_1 \\ m = 2 : & G_2 = \{g_1, g_3\} = C_2 \\ & G_3 = \{g_1, g_5\} \text{ and } G'_3 = \{g_1, g_7\} = C_s^c \\ & G_4 = \{g_1, g_6\} \text{ and } G'_4 = \{g_1, g_8\} = C_s^d \\ m = 4 : & G_5 = \{g_1, g_2, g_3, g_4\} = C_4 \\ & G_6 = \{g_1, g_3, g_5, g_7\} = C_{2v}^c \\ & G_7 = \{g_1, g_3, g_6, g_8\} = C_{2v}^d \\ m = 8 : & G_8 = \{g_1, g_2, g_3, g_4, g_5, g_6, g_7, g_8\} = C_{4v} \end{aligned} \quad (42)$$

Note that throughout this paper, we use Schoenflies notation for the point symmetry groups and distinguish between coordinate and diagonal settings of some subgroups using the superscripts “c” and “d”, respectively.

Let us suppose that the equilibrium state of our molecule is *stable* under arbitrary infinitesimal displacements of the atoms in the xy -plane. Moreover, we will also assume that this state is *isolated* in the sense that within a finite radius neighborhood around it there are no other equilibrium states.

Next, we consider the planar vibrations, i.e. vibrations of the molecule in the plane of its equilibrium configuration. Let us excite a vibrational regime of our molecule by displacing the atoms from their equilibrium positions in a specific manner. As a result of such displacements, the *initial configuration* of the molecule will have a well defined symmetry which is described by one of the *subgroups* of the group G_{4v} listed in (42).

Indeed, the first configuration in Fig. 3 with atoms displaced *arbitrarily* corresponds to the symmetry group $G_1 = C_1$. In this figure, we depict by arrows the atomic displacements and by thin lines the resulting instantaneous configurations of the molecule.

For our analysis, it is essential that the symmetry of the instantaneous configuration of the mechanical system be preserved during the vibrational motions. More precisely, if an atomic pattern at time t_0 has a symmetry element g , this element cannot disappear spontaneously at any $t > t_0$. This proposition, which we call the "symmetry preservation theorem", can be proved rigorously by examining the Hamiltonian equations of motion.

Let us note, however, that spontaneous lowering of the symmetry can occur when the considered dynamical regime *loses its stability* leading most frequently to the appearance of another bush of higher dimension. This important phenomenon, which may be regarded as the dynamical analogue of a phase transition, will be discussed in Section III.

Of course, at the times when all atoms pass through their equilibrium positions, the molecule configuration is again a square. Nevertheless, it can be proved [Sakhnenko & Chechin, 1993] that these isolated instances do not affect such general dynamical properties as the selection rules for excitation transfer between modes of different symmetry.

Thus, all possible vibrational regimes of the square molecule can be classified according to 8 subgroups of the group $G = C_{4v}$. The different configurations of the vibrating molecule, therefore, as depicted in Fig. 3, are the following: a pulsating square ($G_8 = C_{4v}$), a rotating and pulsating square ($G_5 = C_4$), a rectangle ($G_6 = C_{2v}^c$), a rhombus ($G_7 = C_{2v}^d$), a trapezoid ($G_3 = C_s^c$), a deltoid ($G_4 = C_s^d$), a parallelogram ($G_2 = C_2$) or an arbitrary quadrangle ($G_1 = C_1$). All these configurations vary in size as time progresses, but the *type* of the corresponding quadrangle does not change.

Note that the different types of the above vibrational regimes of the molecule are described by *different numbers of degrees of freedom*. Let us discuss this important fact more carefully:

Each of the eight types of vibrational regimes in Fig. 3 corresponds to a certain *bush of NNM's*. For example, the dynamical regime representing a pulsating square ($G = C_{4v}$) can be characterized by only *one* degree of freedom. The edge of the square or the displacement of a certain atom from its equilibrium position along the corresponding diagonal can be used to represent this degree of freedom. Such a vibrational regime is described by a *one-dimensional* bush consisting only of the so-called "breathing" nonlinear normal mode.

The rhombus-type vibration ($G_7 = C_{2v}^d$) and rectangle-type vibration ($G_6 = C_{2v}^c$) are characterized by *two* degrees of freedom. The length of the diagonals in the former case and the length of the adjacent edges in the latter can be chosen as these degrees of freedom. Both of these vibrational regimes are described by *two-dimensional* bushes of modes. Similarly, one can check that a trapezoid-type vibration ($G = C_s^c$) corresponds to a *three-dimensional* bush, the deltoid-type vibration to a *four-dimensional* bush and the vibration with arbitrary quadrangle is represented by a *five-dimensional* bush of vibrational modes. Note that vibrations with $G_5 = C_4$ group are described by a two-dimensional bush consisting of one rotating and one pulsating mode.

Let us also emphasize that the above-discussed classification of vibrational regimes does not depend on the interparticle interactions characterizing the mechanical system. On the other hand, the time-evolution of the degrees of freedom corresponding to a certain bush *does* depend on these interactions in an essential way, as we discuss in more detail below.

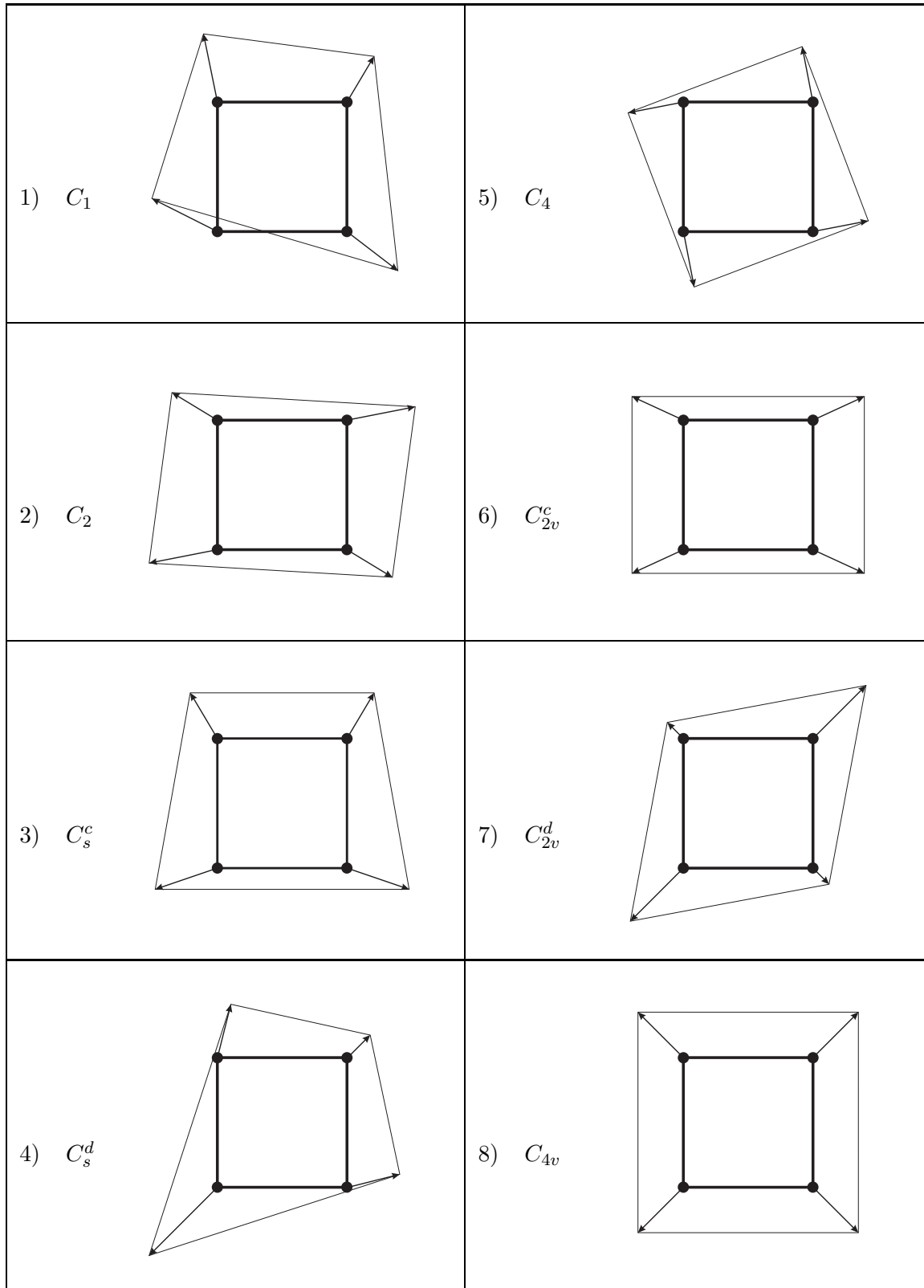


Fig. 3. Different vibrational regimes (bushes of NNMs) of the square molecule.

2.5. Bushes of NNMs for a simple octahedral structure

Finally, let us describe the occurrence of bushes in a 3-dimensional mechanical system consisting of six mass points (called particles or atoms) whose interactions are described by a pair isotropic potential $u(r)$, r being the distance between two particles. We suppose that, at equilibrium, these particles form a regular octahedron with edge a_0 as depicted in Fig. 4. Let us introduce a Cartesian coordinate system. Four particles of the above octahedron lie in the x, y plane and form a square with edge a_0 . Two other particles lie on the z -axis and are called “top particle” and “bottom particle” with respect to the direction of the z -axis. The distance between these particles is also equal to a_0 .

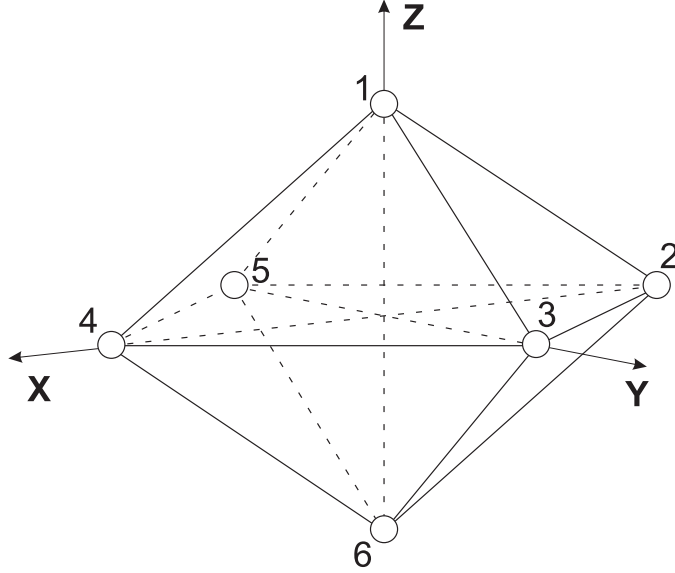


Fig. 4. Octahedral mechanical system.

At equilibrium, this system possesses the point symmetry group O_h and all its possible bushes of vibrational modes are listed in [Chechin *et al.*, 2003]. We may suppose that $u(r)$ is the well-known Lennard-Jones potential:

$$u(r) = \frac{A}{r^{12}} - \frac{B}{r^6}, \quad (43)$$

as we have done in [Chechin *et al.*, 2003], where we studied the stability of the bushes in the octahedral molecule. In the present section, however, we shall consider $u(r)$ as an *arbitrary* pair isotropic potential.

The potential energy of our system in its vibrational state is written in the form

$$U(\vec{X}) = \sum_{\substack{i,j \\ (i < j)}} u(r_{ij}), \quad (44)$$

where r_{ij} is the distance between the i th and j th particles. The N -dimensional vector $\vec{X} = \{x_1(t), x_2(t), \dots, x_N(t)\}$ in Eq. (44) determines the displacements of all particles at an arbitrary chosen instant t . Here $N = 18$ is the total number of degrees of freedom of the octahedral mechanical system.

The configuration vector $\vec{X}(t) = \{x_1(t), x_2(t), \dots, x_{18}(t)\}$ determines all the dynamical variables $x_i(t)$ as follows: The first three components of this vector correspond to the x -, y - and z -displacements of particle 1, the next three components correspond to x -, y -, z -displacements of particle 2, etc., as numbered in Fig. 4. The dynamics of this system is described by Newton's equations

$$\ddot{x}_i = -\frac{\partial U}{\partial x_i}, \quad i = 1, 2, \dots, 18$$

with the masses of all particles equal to unity.

Each bush of modes corresponds to a certain subgroup G_j of the symmetry group $G_0 = O_h$ of the mechanical system at equilibrium. This means that the vibrational state described by the bush possesses the symmetry group $G_j \subset G_0$ and, therefore, there exist certain *restrictions* on the dynamical variables $x_i(t)$. As a result, the number m of degrees of freedom corresponding to the given bush (i.e. its dimension), is smaller than the total number of dynamical variables of the system.

Indeed, at any time t , the atom configuration in a vibrational state represents a polyhedron characterized by the symmetry group $G_j \subset O_h$. Thus, instead of the old variables $x_i(t)$, we introduce m new variables $y_j(t)$ ($j = 1, \dots, m$), which completely determine this polyhedron. Next, we employ the well-known Lagrange method (see, for example, [Landau & Lifshitz, 1976]) for obtaining the dynamical equations in terms of the new variables $y_j(t)$.

For this purpose, we introduce the Lagrange function $L = T - U$, where T is the kinetic and U is the potential energy expressed as functions of new variables y_j and new momenta \dot{y}_j ($j = 1, \dots, m$). Then Euler–Lagrange equations in the new variables read

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{y}_j} \right) - \frac{\partial L}{\partial y_j} = 0, \quad j = 1, \dots, m, \quad (45)$$

where m is the dimension of the considered bush.

We will not present here the tedious derivation of such equations for the octahedral molecule (see e.g. [Chechin *et al.*, 2003], where dynamical equations for bushes are obtained by means of an appropriate MAPLE-program). Rather, we will give the final results for the bushes $B[O_h]$, $B[D_{4h}]$ and $B[C_{4v}]$. Here, in the square brackets next to the bush symbol B , we give the symmetry group of the corresponding bush of vibrational modes. The symmetry groups of the above bushes satisfy the following group-subgroup relations:

$$C_{4v} \subset D_{4h} \subset O_h. \quad (46)$$

The bushes $B[O_h]$, $B[D_{4h}]$, and $B[C_{4v}]$ have one, two and three dimensions, respectively, while their geometrical features can be immediately seen from the symmetry groups that correspond to them. Indeed, the one-dimensional bush $B[O_h]$ consists of only one (“breathing”) mode: The appropriate nonlinear dynamical regime describes the evolution of a regular octahedron whose edge $a = a(t)$ periodically changes in time.

The two-dimensional bush $B[D_{4h}]$ describes a dynamical regime with two degrees of freedom. The symmetry group $G = D_{4h}$ of this bush contains the four-fold axis symmetry coinciding with the z coordinate axis and the mirror plane coinciding with the x, y plane. This symmetry group restricts essentially the shape of the polyhedron describing our mechanical system in the vibrational state. Indeed, the presence of the four-fold axis demands that the quadrangle in the x, y plane be a square. For the same reason, the four edges connecting the particles in the x, y plane (vertices of the above square) with the top particle lying on the z -axis must have the same length, which we denote by $b(t)$.

Similarly, let the length of the edges connecting the bottom particle on the z -axis with any of the four particles in the x, y plane be denoted by $c(t)$. In the case of the bush $B[D_{4h}]$, $b(t) = c(t)$ for any t , because of the presence of the horizontal mirror plane in the group $G = D_{4h}$. However, for the three-dimensional bush $B[C_{4v}]$, this mirror plane is absent and, therefore, $b(t) \neq c(t)$. We illustrate the instantaneous configuration of our mechanical system vibrating according to the bush $B[C_{4v}]$ in Fig. 5.

Let us also introduce the heights, $h_1(t)$ and $h_2(t)$ of the perpendicular distances, respectively, from the top and bottom vertices of our polyhedron onto the x, y plane. We can now write the dynamical equations of the above bushes in terms of the purely geometrical variables $a(t), b(t), c(t), h_1(t)$ and $h_2(t)$.

Choosing $a(t)$ and $h(t) \equiv h_1(t) \equiv h_2(t)$ as suitable variables for describing the two-dimensional bush $B[D_{4h}]$ and $a(t), h_1(t)$ and $h_2(t)$ as appropriate for describing the three-dimensional bush $B[C_{4v}]$, we can write the potential energy for our bushes of vibrational modes as follows:

$$\begin{aligned} B[O_h] : U(a) &= 12u(a) + 3u(\sqrt{2}a), \\ B[D_{4h}] : U(a, h) &= 4u(a) + 2u(\sqrt{2}a) + 8u\left(\sqrt{h^2 + \frac{a^2}{2}}\right) + u(2h), \\ B[C_{4v}] : U(a, h_1, h_2) &= 4u(a) + 2u(\sqrt{2}a) + 4u(b) + 4u(c) + u(h_1 + h_2), \end{aligned}$$

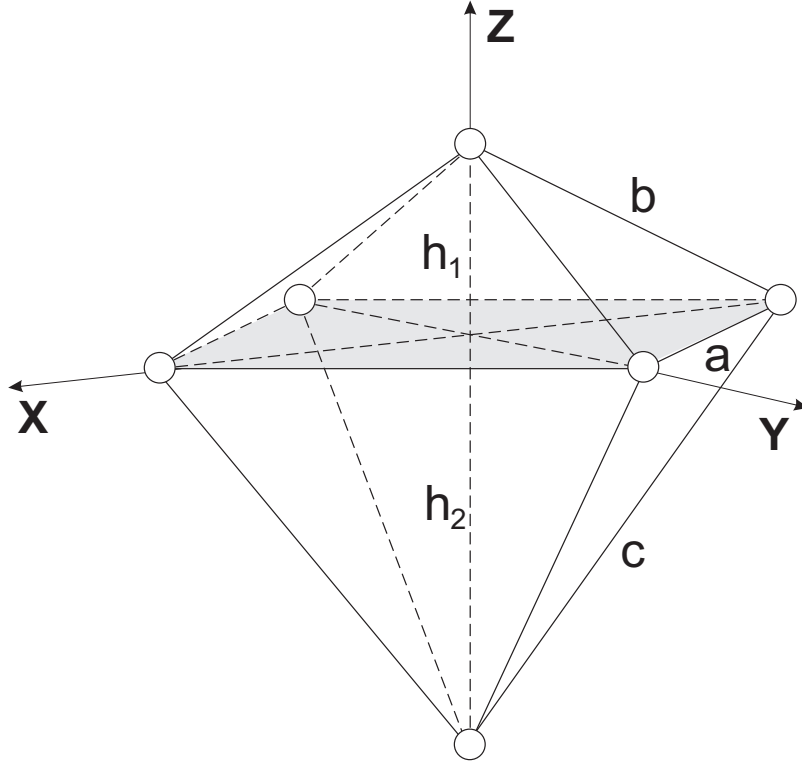


Fig. 5. The distorted octahedron illustrating positions of particles at fixed instant for the bush $B[C_{4v}]$.

where $b = \sqrt{\frac{a^2}{2} + (\frac{5}{4}h_1 - \frac{1}{4}h_2)^2}$, $c = \sqrt{\frac{a^2}{2} + (\frac{5}{4}h_2 - \frac{1}{4}h_1)^2}$.

Then, with the aid of Lagrange's equations, we obtain the following dynamical equations for the above bushes of vibrational modes:

$$\begin{aligned}
 &B[O_h]: \\
 &\quad \ddot{a} = -4u'(a) - \sqrt{2}u'(\sqrt{2}a); \\
 &B[D_{4h}]: \\
 &\quad \ddot{a} = -2u'(a) - \sqrt{2}u'(\sqrt{2}a) - 2u'(b)\frac{a}{b}, \\
 &\quad \ddot{h} = -4u'(b)\frac{h}{b} - u'(2h); \\
 &B[C_{4v}]: \\
 &\quad \ddot{a} = -2u'(a) - \sqrt{2}u'(\sqrt{2}a) - u'(b)\frac{a}{b} - u'(c)\frac{a}{c}, \\
 &\quad \ddot{h}_1 = -u'(b)\frac{5h_1 - h_2}{b} - u'(h_1 + h_2), \\
 &\quad \ddot{h}_2 = -u'(c)\frac{5h_2 - h_1}{c} - u'(h_1 + h_2).
 \end{aligned} \tag{47}$$

Thus, we derive dynamical equations for our bushes of vibrational modes in terms of variables having an explicit geometrical nature. Each bush describes a certain nonlinear dynamical regime corresponding to a vibrational state of the considered mechanical system, so that at any fixed time the configuration of this system is represented by a definite polyhedron characterized by the symmetry group G of the given bush.

The above dynamical equations for the bushes $B[O_h]$, $B[D_{4h}]$ and $B[C_{4v}]$ are *exact*, but rather complicated to solve. One may consider instead some *approximate* equations which can be obtained by expanding the potential energy in Taylor series (near the equilibrium state) keeping only the lowest order terms in the expansion.

Thus, using the first few leading terms in such decompositions, it turns out that bushes belonging to systems of different physical nature, with different symmetry groups and different structures can produce *equivalent dynamical equations*. More precisely, the equations for many bushes can be written in *the same form*, and this fact leads to the idea of the “classes of dynamical universality” mentioned in

[Sakhnenko & Chechin, 1993, 1994; Chechin & Sakhnenko, 1998].

Returning to the dynamical equations (47) for the bushes $B[O_h]$, $B[D_{4h}]$, $B[C_{4v}]$, we see that every bush can be considered as a *reduced* dynamical system whose dimension (m) is less than the full dimension of the considered mechanical system. If the original system is Hamiltonian, the reduced system can also be proved to be Hamiltonian.

3. Bushes of NNMs in modal space and stability analysis

Vectors $\vec{X}(t)$, corresponding to bushes of NNMs, are determined in the configuration space \mathfrak{R}^N . If we introduce in this space a basis set of vectors $\{\vec{\varphi}_1, \vec{\varphi}_2, \dots, \vec{\varphi}_N\}$, the dynamical regime of our mechanical system can be represented by a linear combination of the vectors $\vec{\varphi}_j$ with time dependent coefficients $\nu_j(t)$ as:

$$\vec{X}(t) = \sum_{j=1}^N \nu_j(t) \vec{\varphi}_j \quad (48)$$

where the functions $\nu_j(t)$ entering this decomposition represent *new dynamical variables*.

Every term in the sum (48) has the form of a NNM, whose basis vector $\vec{\varphi}_j$ determines a displacement pattern, while the functions $\nu_j(t)$ determine the time evolution of the atomic displacements. Because of this interpretation, we can consider a given dynamical regime $\vec{X}(t)$ as a *bush* of NNMs. In fact, as will be shown later one often speaks about *root* modes and *secondary* modes of a given bush.

Note that each NNM $\nu_j(t)\vec{\varphi}_j$ from (48) is not, in general, a solution of the dynamical equations of the considered mechanical system, while a specific linear combination of a number of these modes can represent such a solution and, thus describe an exact dynamical regime. Sometimes, for brevity, we will use the word "mode" not only for the whole term $\nu_j(t)\vec{\varphi}_j$, but also for the time dependent function $\nu_j(t)$.

3.1. Normal coordinates and normal modes

Normal coordinates and normal modes are commonly introduced in the theory of *small vibrations* of multiparticle systems (see, for example, [Landau & Lifshitz, 1976]) in the framework of the *harmonic approximation*, where they represent *exact* solutions of the corresponding dynamical equations.

In this approximation, the potential energy $U(\vec{X})$ is decomposed into a Taylor series with respect to the atomic displacements $x_i(t)$ from their equilibrium positions and all terms whose orders are higher than 2 are neglected (because the displacements are supposed to be sufficiently small). As a result, the dynamical equations

$$m_i \ddot{x}_i = -\frac{\partial U}{\partial x_i}, \quad (i = 1, \dots, N) \quad (49)$$

turn out to be *linear differential equations*, with constant coefficients.

Each normal mode is a particular solution to Eq. (49) of the form

$$\vec{X}(t) = \vec{c} \cos(\omega t + \varphi_0), \quad (50)$$

where the N -dimensional constant vector $\vec{c} = \{c_1, c_2, \dots, c_N\}$ and the constant phase φ_0 determine the initial displacements of all particles from their equilibrium state and ω is the frequency of vibration.

Since $U(\vec{X})$ has a quadratic form, substituting (50) into Eq. (49) and dividing the resulting equations by $\cos(\omega t + \varphi_0)$, we reduce the problem of finding the normal modes to the algebraic problem of evaluating the eigenvalues and eigenvectors of the matrix $\mathcal{K} = \|k_{ij}\|$ with coefficients

$$k_{ij} = \frac{\partial^2 U}{\partial x_i \partial x_j} \Big|_{\vec{X}=0} \quad i, j = 1..N. \quad (51)$$

Each eigenvalue of this matrix is the square of the frequency, ω_j^2 , of the j th normal mode, while its eigenvector \vec{c}_j represents the pattern of this normal mode and is called the *normal coordinate*.

Being real and symmetric, the $N \times N$ matrix \mathcal{K} possesses N eigenvectors \vec{c}_j ($j = 1, \dots, N$) and N eigenvalues ω_j^2 . The complete collection of these vectors, i.e. the N normal coordinates, can be used as the *basis* of the configuration space, hence we may write

$$\vec{X}(t) = \sum_{i=1}^N \mu_j(t) \vec{c}_j, \quad (52)$$

where $\vec{X}(t) = \{x_1(t), x_2(t), \dots, x_N(t)\}$, while $\mu_j(t)$ are new dynamical variables which we introduce instead of the old variables $x_i(t)$ ($i = 1, \dots, N$).

If the transformation to normal coordinates is used in the absence of degeneracies, the corresponding system of linear ODEs leads to a set of uncoupled harmonic oscillators

$$\ddot{\mu}_j(t) + \omega_j^2 \mu_j(t) = 0, \quad j = 1, \dots, N$$

with the well-known solution

$$\mu_j(t) = a_j \cos(\omega_j t + \varphi_{0j}), \quad (53)$$

where a_j and φ_{0j} are arbitrary constants.

Note the distinction we make between a *normal coordinate*, represented by the eigenvector \vec{c}_j , and a normal mode, referring to the product of the vector \vec{c}_j and the time-periodic function $\mu_j(t) = \cos(\omega_j t + \varphi_{0j})$.

3.2. *Symmetry-adapted coordinates as basis of the configuration space*

In general, the normal coordinates (normal modes) depend on the interparticle interactions in the mechanical system. Indeed, the concrete form of the potential energy is needed for their construction according to the above-described procedure. Because of this fact, it is more convenient to use *symmetry-adapted* coordinates, instead of normal coordinates. The former are the basis vectors of the *irreducible representations* of a certain parent group. More importantly, the symmetry-adapted coordinates do not depend on the interparticle interactions and can be obtained by the appropriate group theoretical methods.

Note that, for simple mechanical systems, the normal and the symmetry-adapted coordinates may *coincide* with each other. This coincidence is a consequence of the fact that each irreducible representation of the parent group is contained *only once* in the decomposition of the reducible vibrational representation into its irreducible parts.

We complete this part of our study by recalling in Appendix A some notions from the theory of matrix representations of symmetry groups. We also discuss in Appendix A the theory of irreducible representations and describe how they can prove especially helpful in analyzing important problems of crystal vibrations in Solid State Physics.

This concludes our brief outline of the group theoretical concepts needed to find bushes of vibrational modes for arbitrary mechanical systems. The interested reader will find more details in [Sakhnenko & Chechin, 1993; Chechin & Sakhnenko, 1998; Chechin *et al.*, 2000; Chechin, 1989]. Now, it is time to discover how this approach of discrete symmetries can help us analyze the stability properties of the periodic and quasiperiodic solutions belonging to these bushes.

3.3. *Linear stability analysis of bushes of NNMs*

Let us begin by considering individual NNMs, representing one-dimensional bushes of the FPU- β Hamiltonian.

1. *Example 1: Stability of the π -mode in the FPU- β chain*

The question of *local stability* near NNMs of the form \hat{x}_j may be answered by studying the linearized equations about them, setting $x_j = \hat{x}_j + y_j$ and keeping up to linear terms in y_j . For example, in the case of the NNM (8) these equations become ($\beta = 1$):

$$\ddot{y}_j = (1 + 48\hat{x}^2)(y_{j-1} - 2y_j + y_{j+1}), \quad j = 1, \dots, N \quad (54)$$

where \hat{x} is the solution of (9), see also equations (10)-(13), and $y_1 = y_{N+1}$, $y_0 = y_N$, due to p.b.c..

According to Floquet theory, linear stability analysis of periodic solutions is performed by studying the eigenvalues of the monodromy matrix $M(T)$, whose N columns are the fundamental solutions of Eq.(54) evaluated at $t = T$ (the period of the NNM), with $M(0)$ equal to the $N \times N$ identity matrix. However, in the case of such simple modes as (8), it is much easier to diagonalize first the variational equations into N uncoupled Lamé equations

$$\ddot{z}_j(t) + 4(1 + 48\hat{x}^2)\sin^2\left(\frac{\pi j}{2N}\right)z_j(t) = 0, \quad j = 1, \dots, N \quad (55)$$

where the z_j variations are simple linear combinations of the y_j 's. Changing variables to $u = \lambda t$, where $\lambda^2 = 4/(1 - 2k^2)$ and using (10)-(13) this equation takes the form

$$z_j''(u) + (1 + 22k^2 - 24k^2 \operatorname{sn}^2(u, k^2))\sin^2\left(\frac{\pi j}{2N}\right)z_j(u) = 0, \quad j = 1, \dots, N \quad (56)$$

where primes denote differentiation with respect to u . Equation (56) is an example of Hill's equation

$$z''(u) + Q(u)z(u) = 0 \quad (57)$$

where $Q(u)$ is a T -periodic function ($Q(u) = Q(u + T)$). According to Floquet theory, its solutions are bounded or unbounded depending on whether the eigenvalues of its monodromy matrix lie on the unit circle or not. The first variation $z_j(u)$ to become unbounded as $k \geq k_c$ determines the total energy of the lattice

$$E_c = \frac{Nk_c^2 + 2Nk_c^4}{(1 - 2k_c^2)^2} \quad (58)$$

at which this particular NNM becomes unstable for $0 \leq k \leq \frac{1}{\sqrt{2}}$

2. Example 2: Stability of the π -mode in the FPU- α chain

Let us consider the stability of the one-dimensional bush $B[\hat{a}^2, \hat{i}]$, representing the π -mode, in the FPU- α chain with $N = 4$ particles under p.b.c.

The equations for this nonlinear chain read

$$\begin{aligned} \ddot{x}_1 &= f(x_2 - x_1) - f(x_1 - x_4), \\ \ddot{x}_2 &= f(x_3 - x_2) - f(x_2 - x_1), \\ \ddot{x}_3 &= f(x_4 - x_3) - f(x_3 - x_2), \\ \ddot{x}_4 &= f(x_1 - x_4) - f(x_4 - x_3), \end{aligned} \quad (59)$$

where $f(x) = x + \alpha x^2$. Clearly, the π -mode represents here the exact *periodic* vibrational regime $\vec{X} = \{A(t), -A(t), A(t), -A(t)\}$, with $A(t) = C_0 \cos(2t)$. According to the conventional prescription, we should linearize the dynamical system (59) in the neighborhood of the given bush and study the resulting system of ODEs. To achieve this, we write

$$\vec{X}(t) = \vec{C}(t) + \vec{\delta}(t), \quad (60)$$

where $\vec{C} = \{A(t), -A(t), A(t), -A(t)\}$ is our NNM, while $\vec{\delta}(t) = \{\delta_1(t), \delta_2(t), \delta_3(t), \delta_4(t)\}$ is an infinitesimal vector. Substituting (60) into Eqs. (59) with $f(x) = x + x^2$ (i.e. $\alpha = 1$) and neglecting all terms nonlinear in $\delta_j(t)$, we obtain for this FPU- α model the system of linearized equations:

$$\ddot{\vec{\delta}} = \mathcal{J}(t)\vec{\delta}, \quad (61)$$

where $\mathcal{J}(t)$ is the *Jacobi* matrix of (59) for the FPU- α chain calculated by the substitution of the vector $\vec{X} = \vec{C} = \{A(t), -A(t), A(t), -A(t)\}$. This matrix can be expressed as follows:

$$\mathcal{J}(t) = \mathcal{L} + 4A(t)\mathcal{M}, \quad (62)$$

where

$$\mathcal{L} = \begin{pmatrix} -2 & 1 & 0 & 1 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 1 & 0 & 1 & -2 \end{pmatrix}, \quad \mathcal{M} = \begin{pmatrix} 0 & -1 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \end{pmatrix} \quad (63)$$

are time-independent symmetric matrices.

It is easy to verify that \mathcal{L} and \mathcal{M} commute with each other; therefore, there exists a time-independent orthogonal matrix \mathcal{S} transforming both \mathcal{L} and \mathcal{M} into diagonal form: $\tilde{\mathcal{S}}\mathcal{L}\mathcal{S} = \mathcal{L}_{dia}$, $\tilde{\mathcal{S}}\mathcal{M}\mathcal{S} = \mathcal{M}_{dia}$ (where $\tilde{\mathcal{S}}$ is the transpose of \mathcal{S}). In turn, this means that the Jacobi matrix $\mathcal{J}(t)$ can be diagonalized at *any time* t by one and the same *time-independent* matrix \mathcal{S} . Therefore, our linearized system (61) for the considered bush $B[\hat{a}^2, \hat{\mathbf{i}}]$ can be decomposed into four *independent* differential equations.

Observe that, due to similar reasons, we were able to reduce (54) into a system of N uncoupled ODEs, see (55), for the π - mode of the FPU β - chain in Example 1.

The above matrix \mathcal{S} can be obtained with the aid of the theory of irreducible representations of the symmetry group G , for the case $G = D_2$ considered here. The general method for obtaining the matrix \mathcal{S} uses the basis vectors of irreducible representations of the group G , constructed in the mechanical space of the considered dynamical system. In the simple example of a monoatomic chain with $N = 4$ particles, this method leads to the following result

$$\mathcal{S} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}. \quad (64)$$

The rows of the matrix \mathcal{S} in (64) are simply the characters of four one-dimensional irreducible representations (irreps) – $\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4$ – of the Abelian group D_2 , because each of these irreps is contained once in the decomposition of the natural representation of the group $G = D_2$ (see also Appendix A). Introducing new variables $\vec{Y} = \{y_1, y_2, y_3, y_4\}$ by the transformation $\vec{Y} = \mathcal{S}\vec{\delta}$, with \mathcal{S} as in (64), we arrive at the *complete splitting* of the linearized equations (61) for the FPU- α model:

$$\ddot{y}_1 = 0, \quad (65a)$$

$$\ddot{y}_2 = -2[1 + 4A(t)]y_2, \quad (65b)$$

$$\ddot{y}_3 = -4y_3, \quad (65c)$$

$$\ddot{y}_4 = -2[1 - 4A(t)]y_4, \quad (65d)$$

where $A(t) = C_0 \cos(2t)$.

With the aid of Eqs. (65) one can now determine precisely the threshold value for C_0 , leading to the loss of stability of the one-dimensional bush $B[\hat{a}^2, \hat{\mathbf{i}}]$. Indeed, according to Eqs. (65), the variables $y_j(t)$ ($j = 1, 2, 3, 4$) are independent from each other, and we can solve for them separately: Eq. (65a) for $y_1(t)$ describes the uniform motion of the center of mass of our chain, since it follows from the equations $\vec{Y} = \mathcal{S}\vec{\delta}$ that $y_1(t) = (\delta_1(t) + \delta_2(t) + \delta_3(t) + \delta_4(t))/2$. Therefore, considering *vibrational* regimes only, we may assume $y_1(t) \equiv 0$.

If, in the solution of the system (65), $y_j(t) = 0$ for $j = 1, 2$ but not $j = 3$, $\vec{\delta} = \tilde{\mathcal{S}}\vec{Y}$ would imply (since \mathcal{S} is orthogonal and $\mathcal{S}^{-1} = \tilde{\mathcal{S}}$): $\vec{\delta}(t) = \{y_3(t), -y_3(t), y_3(t), -y_3(t)\}$, where $y_3(t) \sim \cos(2t)$. This leads to variations “along” the bush $\vec{X}(t) = C_0\{\cos(2t), -\cos(2t), \cos(2t), -\cos(2t)\}$, which do not affect the stability of the motion.

On the other hand, if $y_2(t)$ and $y_4(t)$ are nonzero, with $A(t) = C_0 \cos(2t)$, Eq. (65b) and (65d) imply $\ddot{y}_j + [2 + 8C_0 \cos(2t)]y_j = 0, j = 2, 4$ and can thus be transformed to the standard form of Mathieu’s equation [Abramowitz & Stegun, 1965]. Therefore, the stability threshold of the considered bush $B[\hat{a}^2, \hat{\mathbf{i}}]$ for $N = 4$ can be determined directly from the well-known diagrams of stable and unstable motion of the Mathieu equation. In this way we find that the lowest critical value $C_c > 0$ of the amplitude C_0 at which the given bush loses its stability is $C_c \approx 0.303$.

Let us now consider the FPU- α chain with $N = 6$ particles. Linearizing the dynamical equations of the FPU- α chain with $N = 6$ in the vicinity of the bush $B[\hat{a}^2, \hat{1}]$ (π -mode), we also obtain a Jacobi matrix of the form (62). However, unlike the case $N = 4$, matrices \mathcal{L} and \mathcal{M} , *do not* commute with each other. As a consequence, *we cannot diagonalize* both matrices \mathcal{L} and \mathcal{M} , i.e. with one and the same orthogonal matrix \mathcal{S} . Thus, it is impossible to diagonalize the Jacobi matrix $\mathcal{J}(t)$ in equation $\ddot{\vec{\delta}} = \mathcal{J}(t)\vec{\delta}$ for all time t . This means that there is no matrix \mathcal{S} that completely decouples the linearized system for the bush $B[\hat{a}^2, \hat{1}]$ for the chain with $N = 6$ particles.

This difference between the cases $N = 4$ and $N = 6$ (generally, for $N > 4$) can be explained group-theoretically as follows: The group $G = [\hat{a}^2, \hat{1}]$ of the considered bush leads to *different* groups for the cases $N = 4$ and $N = 6$. Indeed, for $N = 4$ $[\hat{a}^2, \hat{1}] \equiv \{\hat{e}, \hat{a}^2, \hat{1}, \hat{a}^2\hat{1}\} = D_2$, while for $N = 6$ $[\hat{a}^2, \hat{1}] \equiv \{\hat{e}, \hat{a}^2, \hat{a}^4, \hat{1}, \hat{a}^2\hat{1}, \hat{a}^4\hat{1}\} = D_3$. Group D_3 , on the other hand, is *non-Abelian* ($\hat{1}\hat{a}^4 = \hat{a}^2\hat{1}$), unlike group D_2 ($\hat{1}\hat{a}^2 = \hat{a}^2\hat{1}$) and, as a consequence, possesses not only one-dimensional, but also two-dimensional irreps. This is precisely why we are not permitted to completely decouple the above linearized system² (see [Chechin & Zhukov, 2006]).

In spite of this difficulty, we can still simplify the linearized system $\ddot{\vec{\delta}} = \mathcal{J}(t)\vec{\delta}$ considerably using group theoretical methods (see [Chechin & Zhukov, 2006; Chechin *et al.*, 2007]). Let us present the final result of this splitting for the case $N = 6$:

$$\ddot{y}_1 = -4y_1, \quad (66a)$$

$$\ddot{y}_2 = 0, \quad (66b)$$

$$\begin{cases} \ddot{y}_3 + 2y_3 = P(t)y_5, \\ \ddot{y}_5 + 2y_5 = \bar{P}(t)y_3, \end{cases} \quad (66c)$$

$$\begin{cases} \ddot{y}_4 + 2y_4 = P(t)y_6, \\ \ddot{y}_6 + 2y_6 = \bar{P}(t)y_4. \end{cases} \quad (66d)$$

Here $P(t) = e^{\frac{i\pi}{3}} - 4A(t)[1 + e^{-\frac{i\pi}{3}}]$, while $\bar{P}(t)$ is the complex conjugate of $P(t)$.

The stability of the π -mode (the bush $B[\hat{a}^2, \hat{1}]$) has already been extensively discussed in a number of papers [Budinsky & Bountis, 1983; Sandusky & Page, 1994; Flach, 1996; Chechin *et al.*, 2002, 2005; Poggi & Ruffo, 1997; Yoshimura, 2004; Shinohara, 2002, 2003; Leo & Leo, 2007; Dauxois *et al.*, 2005] by different methods and with emphasis on different aspects of stability. In the papers [Chechin *et al.*, 2002], [Chechin *et al.*, 2005] the stability of all one-dimensional and two-dimensional bushes of vibrational modes, in both FPU- α and FPU- β models was numerically studied. In particular, this study revealed a remarkable property of the FPU- α chain: the stability threshold of the π -mode turns out to be *one and the same* when it interacts with *any* other mode of the chain. By contrast, other nonlinear normal modes of the FPU- α (or FPU- β) chain exhibit very different stability thresholds when interacting with different modes [Chechin *et al.*, 2005].

3.4. Bushes of NNMs in monoatomic chains

To study bushes of NNMs in monoatomic chains, we shall choose the complete set of normal coordinates $\vec{\varphi}_k$ as the basis of the configuration space. Here, we use the normal coordinates in the form presented in [Poggi & Ruffo, 1997]:

$$\vec{\varphi}_k = \left\{ \frac{1}{\sqrt{N}} \left[\sin\left(\frac{2\pi k}{N}n\right) + \cos\left(\frac{2\pi k}{N}n\right) \right] \mid n = 1, \dots, N \right\}, \quad k = 0..N-1, \quad (67)$$

where the subscript k refers to the mode and the subscript n refers to the atom. The vectors $\vec{\varphi}_k$ ($k = 0, 1, 2, \dots, N-1$) form an orthonormal basis, in which we can expand the set of atomic displacements $\vec{X}(t)$

²Actually, this fact can be understood if one takes into account that the two-dimensional irrep is contained two times in the decomposition of the natural representation of the considered chain.

corresponding to a given bush as follows:

$$\vec{X}(t) = \sum_{k=0}^{N-1} \nu_k(t) \vec{\varphi}_k. \quad (68)$$

For example, one obtains the following expressions for the bushes $B[\hat{a}^4, \hat{1}]$ and $B[\hat{a}^4, \hat{a}^2 \hat{1}]$ [see Eqs. (35), (37)]:

$$\begin{aligned} B[\hat{a}^4, \hat{1}] : \quad \vec{X}(t) &= \{ x_1(t), x_2(t), -x_1(t), -x_2(t) \mid x_1(t), x_2(t), -x_1(t), -x_2(t) \mid \cdots \} \\ &= \mu(t) \vec{\varphi}_{N/2} + \nu(t) \vec{\varphi}_{3N/4}, \end{aligned} \quad (69)$$

$$B[\hat{a}^4, \hat{a}^2 \hat{1}] : \quad \vec{X}(t) = \tilde{\mu}(t) \vec{\varphi}_{N/2} + \tilde{\nu}(t) \vec{\varphi}_{N/4}. \quad (70)$$

From the complete basis (67) only the vectors

$$\vec{\varphi}_{N/2} = \frac{1}{\sqrt{N}}(-1, 1, -1, 1, -1, 1, -1, 1, -1, 1, -1, 1, \dots), \quad (71)$$

$$\vec{\varphi}_{N/4} = \frac{1}{\sqrt{N}}(1, -1, -1, 1, 1, -1, -1, 1, 1, -1, -1, 1, \dots), \quad (72)$$

$$\vec{\varphi}_{3N/4} = \frac{1}{\sqrt{N}}(-1, -1, 1, 1, -1, -1, 1, 1, -1, -1, 1, 1, \dots). \quad (73)$$

contribute to the two-dimensional bushes (69), (70), which are equivalent to each other and constitute an examples of dynamical domains. For the bush $B[\hat{a}^4, \hat{1}]$, we can find the following relations between the old dynamical variables $x_1(t)$, $x_2(t)$ (corresponding to the configuration space) and the new dynamical variables $\mu(t)$, $\nu(t)$ (corresponding to the modal space):

$$\begin{aligned} \mu(t) &= -\frac{\sqrt{N}}{2}[x_1(t) - x_2(t)], \\ \nu(t) &= -\frac{\sqrt{N}}{2}[x_1(t) + x_2(t)]. \end{aligned} \quad (74)$$

Thus, each of the above bushes consists of two modes. One of these modes is the *root* mode ($\vec{\varphi}_{3N/4}$ for the bush $B[\hat{a}^4, \hat{1}]$ and $\vec{\varphi}_{N/4}$ for the bush $B[\hat{a}^4, \hat{a}^2 \hat{1}]$), while the other mode $\vec{\varphi}_{N/2}$ is the *secondary* mode. Indeed, according to [Sakhnenko & Chechin, 1993; Chechin & Sakhnenko, 1998] the *symmetry* of the *secondary modes* must be *higher or equal* to the symmetry of the root mode. In our case, as we deduce from Eq. (72), the translational symmetry of the mode $\vec{\varphi}_{N/4}$ is \hat{a}^4 (acting by this element on (72) produces the same displacement pattern), while the translational symmetry of the mode $\vec{\varphi}_{N/2}$ is \hat{a}^2 , which has twice more symmetry elements than that of $\vec{\varphi}_{N/4}$ [see (71), (72)]. Note that the *full* symmetry of the modes $\vec{\varphi}_{N/4}$ and $\vec{\varphi}_{N/2}$ is represented by $[\hat{a}^4, \hat{a}^2 \hat{1}]$ and $[\hat{a}^2, \hat{1}]$, respectively.

Let us now return to the Hamiltonian of the FPU system written as follows:

$$H = T + V = \frac{1}{2} \sum_{n=1}^N \dot{x}_n^2 + \frac{1}{2} \sum_{n=1}^N (x_{n+1} - x_n)^2 + \frac{\gamma}{p} \sum_{n=1}^N (x_{n+1} - x_n)^p. \quad (75)$$

Here $p = 3$, $\gamma = \alpha$ for the FPU- α chain, and $p = 4$, $\gamma = \beta$ for the FPU- β chain, while T and V are the kinetic and potential energies, respectively. We assume again p.b.c.

Let us consider the set of atomic displacements corresponding to the two-dimensional bush $B[\hat{a}^4, \hat{1}]$

$$\vec{X}(t) = \{ x, y, -y, -x \mid x, y, -y, -x \mid x, y, -y, -x \mid \cdots \}, \quad (76)$$

where we rename $x_1(t)$ and $x_2(t)$ from Eq. (69) as $x(t)$ and $y(t)$, respectively. Substituting the atomic displacements from Eq. (76) into the Hamiltonian (75) corresponding to the FPU- α chain we obtain:

$$T = \frac{N}{4}(\dot{x}^2 + \dot{y}^2), \quad (77)$$

$$V = \frac{N}{4}(3x^2 - 2xy + 3y^2) + \frac{N\alpha}{2}(x^3 + x^2y - xy^2 - y^3). \quad (78)$$

These expressions are valid for an arbitrary FPU- α chain with $N \bmod 4 = 0$. The size of the extended primitive cell (EPC) for the vibrational state (76) is equal to $4a$ and, therefore, when calculating the

energies T and V , we may restrict ourselves to summing over only one EPC. In the present case, Lagrange's equations (45) can be written as follows:

$$\begin{cases} \ddot{x} + (3x - y) + \alpha(3x^2 + 2xy - y^2) = 0, \\ \ddot{y} + (3y - x) + \alpha(x^2 - 2xy - 3y^2) = 0. \end{cases} \quad (79)$$

Let us emphasize that these equations do not depend on the number N of the particles in the chain (only $N \bmod 4 = 0$ must hold).

Eqs. (79) are written in terms of the atomic displacements $x(t)$ and $y(t)$. From them, it is easy to obtain the dynamical equations for the bush *in terms of the normal modes* $\mu(t)$ and $\nu(t)$. Using the relations (74) between the old and new variables, we find the following equations for the bush $B[\hat{a}^4, \hat{1}]$ in the modal space

$$\ddot{\mu} + 4\mu - \frac{4\alpha}{\sqrt{N}}\nu^2 = 0, \quad (80)$$

$$\ddot{\nu} + 2\nu - \frac{8\alpha}{\sqrt{N}}\mu\nu = 0. \quad (81)$$

The Hamiltonian for the bush $B[\hat{a}^4, \hat{1}]$, considered as a two-dimensional dynamical system, can be written in the modal space as follows:

$$H[\hat{a}^4, \hat{1}] = \frac{1}{2}(\dot{\mu}^2 + \dot{\nu}^2) + (2\mu^2 + \nu^2) - \frac{4\alpha}{\sqrt{N}}\mu\nu^2. \quad (82)$$

Note that dynamical equations for all one-dimensional and two-dimensional bushes of vibrational modes for the FPU-chains were presented in [Chechin *et al.*, 2005].

3.5. Stability of bushes of vibrational modes in nonlinear chains

3.5.1. Consideration in modal space

Since the term “stability” is often used in the literature with different meanings, let us explain in what sense we use it in the present paper.

The stability of bushes of modes was discussed, in general, in [Sakhnenko & Chechin, 1993; Chechin & Sakhnenko, 1998], while in the case of the FPU chains it was considered in [Chechin *et al.*, 2002, 2005]. Following these papers, we also discuss here the stability of a given bush of normal modes with respect to its interactions³ with the modes which *do not belong* to this bush. Let us illustrate this idea with an example.

As was shown above, the two-dimensional bush $B[\hat{a}^4, \hat{1}]$ for the FPU- α chain is described by Eqs. (80),(81). These equations admit a special solution of the form

$$\mu(t) \neq 0, \quad \nu(t) \equiv 0. \quad (83)$$

which can be excited by imposing the initial conditions: $\mu(t_0) = \mu_0 \neq 0$, $\dot{\mu}(t_0) = 0$, $\nu(t_0) = 0$, $\dot{\nu}(t_0) = 0$. Substitution of (83) into (80) produces the dynamical equation of the one-dimensional bush $B[\hat{a}^2, \hat{1}]$ (see [Chechin *et al.*, 2005]) consisting of only one mode $\mu(t)$

$$\ddot{\mu} + 4\mu = 0 \quad (84)$$

with the simple solution

$$\mu(t) = \mu_0 \cos(2t). \quad (85)$$

taking (with no loss of generality) the initial phase to be equal to zero. Substituting (85) into Eq. (81), we obtain

$$\ddot{\nu} + \left[2 - \frac{8\alpha\mu_0}{\sqrt{N}} \cos(2t) \right] \nu = 0. \quad (86)$$

³There is an essential difference between the interactions of the modes that belong and those that do not belong to a given bush: we speak about “force interaction” in the former case and about “parametric interaction” in the last case (see [Chechin & Sakhnenko, 1998]).

This equation can be easily transformed into the standard form of the Mathieu equation [Abramowitz & Stegun, 1965]

$$\ddot{\nu} + [a - 2q \cos(2t)]\nu = 0. \quad (87)$$

As is well-known, there exist domains of stable and unstable motion of the Mathieu equation (87) in the $a - q$ plane of its parameters [Abramowitz & Stegun, 1965]. The one-dimensional bush $B[\hat{a}^2, \hat{\mathbf{i}}]$ is stable for sufficiently small amplitudes μ_0 of the mode $\mu(t)$, but becomes unstable when $\mu_0 > 0$ is increased. This phenomenon, similar to the well-known parametric resonance, takes place at μ_0 values which lie within the domains of unstable motion of Mathieu's equation (86).

The loss of stability of the dynamical regime (83), representing the bush $B[\hat{a}^2, \hat{\mathbf{i}}]$, manifests itself in the exponential growth of the mode $\nu(t)$, which was identically zero for the vibrational state (83) and oscillatory for the stable regime of (87). As a result of $\nu(t) \neq 0$, the *dimension* of the original one-dimensional bush $B[\hat{a}^2, \hat{\mathbf{i}}]$ increases and the bush is transformed into the two-dimensional bush $B[\hat{a}^4, \hat{\mathbf{i}}]$. This is accompanied by the *breaking of the symmetry* of the vibrational state (the symmetry of the bush $B[\hat{a}^2, \hat{\mathbf{i}}]$ is twice as high as that of the bush $B[\hat{a}^4, \hat{\mathbf{i}}]$).

In general, we may view a given bush as a stable dynamical object if the *complete collection of its modes* (and, therefore, its dimension) *does not change in time*. All other modes of the system—according to the definition of a bush as a full collection of active modes—possess zero amplitudes and are therefore called “sleeping” modes. If we increase the intensity of bush vibrations, some sleeping modes (because of parametric interactions with the active modes [Chechin & Sakhnenko, 1998]) can lose their stability and become excited. In this situation, we speak of the *loss of stability* of the *original bush*, since the dimension of the vibrational state (the number of active modes) becomes larger, while its symmetry becomes lower. Thus, as a consequence of stability loss, the original bush transforms into another bush of higher dimension. In Section IV we will discuss in more detail the problem of stability of invariant tori from a more general perspective, when we study quasiperiodic orbits in which all modes may be active.

Note, however, that what we described above is the loss of stability of the (one-dimensional) bush $B[\hat{a}^2, \hat{\mathbf{i}}]$ with respect to its transformation into the (two-dimensional) bush $B[\hat{a}^4, \hat{\mathbf{i}}]$, using Floquet theory and analyzing a simple Mathieu's equation. In the case of a more general perturbation of the N particles though, one must examine the stability of the bush $B[\hat{a}^4, \hat{\mathbf{i}}]$ with respect to *all other* modes, as well. This cannot be done using Floquet theory as the variations that need to be studied are *not* about a periodic but a *quasiperiodic* orbit with two rationally independent frequencies. The stability analysis of a multidimensional bush is described theoretically in the next subsection and is performed efficiently and accurately employing the GALI numerical method outlined in section IV.

Indeed, as we shall show in Section IV, it is possible that tori may continue to exist at energies *higher* than the thresholds (obtained by Floquet theory) where their “parent” modes become linearly unstable. This ensures stability over a wider domain than just an infinitesimal neighborhood of the simple periodic orbits (one-dimensional bushes) representing the NNM's of the FPU chain.

3.6. *Stability of bushes of NNMs in the general case*

3.6.1. *Some general comments*

Some aspects of bush stability analysis have already been discussed in the previous sections. In this last subsection of Section III, we would like to complete the discussion of bush stability using the apparatus of the irreducible representations of symmetry groups.

In [Chechin & Zhukov, 2006], a general group theoretical procedure was developed for simplifying the linear stability analysis of periodic and quasiperiodic nonlinear regimes in N -particle mechanical systems with arbitrary groups of discrete symmetry.

This procedure allows us to split the *linearized* equations (near a given dynamical regime) into a number of *independent* subsystems whose dimensions can be much smaller than that of the full system. The basis vectors of the irreducible representations of the appropriate groups are needed to perform this splitting explicitly. On the other hand, we can obtain more easily very useful “splitting schemes”, which

determine how many subsystems of different dimensions can appear as a result of the above splitting with the aid of the group-representation *characters* only. Let us discuss these problems in more detail.

In general, the study of stability of periodic and, especially, quasiperiodic dynamical regimes of mechanical systems with many degrees of freedom presents considerable difficulties. Indeed, for this purpose, we often need to integrate large linearized systems of differential equations with time-dependent coefficients. In the case of a periodic regime, one can use the Floquet approach, which requires integration over only one time-period to construct the monodromy matrix. However, for quasiperiodic regimes this method is not applicable, and one needs to solve a system of several differential equations for very long times in order to detect stability (especially, near an instability threshold).

In such a situation, a decomposition (splitting) of the full linearized system into a number of independent subsystems of small dimensions proves to be very useful. Moreover, this decomposition can provide valuable information regarding the specific degrees of freedom, which are responsible for the first destabilization of a dynamical regime as the energy (or a parameter value) is increased. We remark that the number of such “critical” degrees of freedom can frequently be rather small.

3.6.2. Main theorem of bush stability

Let us consider an N -degrees-of-freedom mechanical system described by the set of autonomous differential equations

$$\ddot{\vec{X}} = \vec{F}(\vec{X}), \quad (88)$$

where the configuration vector $\vec{X} = \{x_1(t), x_2(t), \dots, x_N(t)\}$ determines the deviation from the equilibrium state $\vec{X} = \{0, 0, \dots, 0\}$, while the vector-function $\vec{F}(\vec{X}) = \{f_1(\vec{X}), f_2(\vec{X}), \dots, f_N(\vec{X})\}$ provides the right-hand-side of the dynamical equations.

We assume that Eq. (88) is invariant under the action of a discrete symmetry parent group G_0 . This means that for all $g \in G_0$ Eq. (88) is invariant under the transformation of variables

$$\tilde{\vec{X}} = \hat{g}\vec{X}, \quad (89)$$

where \hat{g} is the operator associated with the symmetry element g of the group G_0 by the conventional definition.

Using (88) and (89), we may write $\vec{X} = \hat{g}^{-1}\tilde{\vec{X}}$, $\hat{g}^{-1}\ddot{\vec{X}} = \ddot{\vec{F}}(\hat{g}^{-1}\tilde{\vec{X}})$, and finally

$$\ddot{\vec{X}} = \hat{g}\vec{F}(\hat{g}^{-1}\tilde{\vec{X}}). \quad (90)$$

On the other hand, renaming \vec{X} from Eq. (88) as $\tilde{\vec{X}}$, one can write $\ddot{\vec{X}} = \vec{F}(\tilde{\vec{X}})$. Comparing this equation with Eq. (90), yields $\vec{F}(\tilde{\vec{X}}) = \hat{g}\vec{F}(\hat{g}^{-1}\tilde{\vec{X}})$, or

$$\vec{F}(\hat{g}\vec{X}) = \hat{g}\vec{F}(\vec{X}). \quad (91)$$

This is the invariance condition of the dynamical equations (88) under the action of the operator \hat{g} . Note that it must hold for all $g \in G_0$, hence it is sufficient to consider such equivalence only for the *generators* of the group G_0 .

Let $\vec{X}(t) = \vec{C}(t)$ be an m -dimensional specific dynamical regime in the considered mechanical system that corresponds to the bush $B[G]$ ($G \subseteq G_0$). This means that there exist functional relations between the individual displacements $x_i(t)$ ($i = 1, 2, \dots, N$), which reduce system (88) to m ODEs in terms of independent functions denoted by $a(t)$, $b(t)$, $c(t)$, etc. in the previous section.

The vector $\vec{C}(t)$ is, therefore, a general solution of the equation [see, Eq. (A.18) in Appendix A]

$$\hat{G}\vec{X} = \vec{X},$$

where G is the symmetry group of the given bush $B[G]$ ($G \subseteq G_0$).

Suppose now we wish to study the *stability* of the dynamical regime $\vec{C}(t)$, corresponding to the bush $B[G]$. To this end, we must linearize the dynamical equations (88) in a vicinity of the given bush, or more precisely, in a vicinity of the vector $\vec{C}(t)$. Thus, let

$$\vec{X} = \vec{C}(t) + \vec{\delta}(t), \quad (92)$$

where $\vec{\delta}(t) = \{\delta_1(t), \dots, \delta_N(t)\}$ is an infinitesimal N -dimensional vector. Substituting $\vec{X}(t)$ from (92) into (88) and linearizing these equations with respect to $\vec{\delta}(t)$, we obtain

$$\ddot{\vec{\delta}} = \mathcal{J}[\vec{C}(t)]\vec{\delta}, \quad (93)$$

where $\mathcal{J}[\vec{C}(t)]$ is the Jacobi matrix of the system (88):

$$\mathcal{J}[\vec{C}(t)] = \left\| \frac{\partial f_i}{\partial x_j} \Big|_{\vec{X}=\vec{C}(t)} \right\|.$$

In [Chechin & Zhukov, 2006], we have proved the following theorem:

Theorem 1. *The matrix $\mathcal{J}[\vec{C}(t)]$ of the linearized dynamical equations near a given bush $B[G]$, determined by the configuration vector $\vec{C}(t)$, commutes with all matrices $\mathcal{M}(g)$ ($g \in G$) of the natural representation of the symmetry group G of the considered bush:*

$$\mathcal{M}(g)\mathcal{J}[\vec{C}(t)] = \mathcal{J}[\vec{C}(t)]\mathcal{M}(g).$$

We introduce, hereafter, a simpler notation for the Jacobi matrix:

$$\mathcal{J}[\vec{C}(t)] \equiv \mathcal{J}(t). \quad (94)$$

Remark. Theorem 1 suggests that if we take a symmetry element $g \in G_0$ that is not contained in G ($g \in G_0 \setminus G$), the matrix \mathcal{M}_g corresponding to g may not commute with $\mathcal{J}(t)$.

Based on the above, we can now apply the well-known Wigner theorem (see, for example, [Elliott & Dawber, 1979]) to split the linearized system $\ddot{\vec{\delta}} = \mathcal{J}(t)\vec{\delta}$ into a number of independent subsystems. In fact, it is useful to formulate this theorem in a way that is convenient for our present purposes.

Consider a reducible representation Γ of the group G which can be decomposed into a direct sum of the irreducible representations (irreps) Γ_j of this group:

$$\Gamma = \sum_j^{\oplus} m_j \Gamma_j. \quad (95)$$

Here m_j is the number of times that Γ_j enters into this decomposition (subduction frequency). We denote the dimension of the irrep Γ_j by n_j . Then the Wigner theorem asserts the following:

Theorem 2. *Any matrix \mathcal{H} commuting with all the matrices of a representation Γ of the group G can be reduced to the block-diagonal form*

$$\mathcal{H} = \sum^{\oplus} \mathcal{D}_j \quad (96)$$

so that: (a) the dimension of the each block \mathcal{D}_j is equal to $m_j n_j$ and (b) the block \mathcal{D}_j consists of sub-blocks representing matrices proportional to the identity matrix \mathcal{I}_{n_j} of dimension n_j which are repeated m_j times along the rows and columns of the block \mathcal{D}_j .

The structure of one such block $\mathcal{D}_j = \mathcal{D}$ characterized by the numbers $n_j = n$, $m_j = m$ is as follows:

$$\mathcal{D} = \begin{pmatrix} \mu_{11}\mathcal{I}_n & \mu_{12}\mathcal{I}_n & \dots & \mu_{1m}\mathcal{I}_n \\ \mu_{21}\mathcal{I}_n & \mu_{22}\mathcal{I}_n & \dots & \mu_{2m}\mathcal{I}_n \\ \dots & \dots & \dots & \dots \\ \mu_{m1}\mathcal{I}_n & \mu_{m2}\mathcal{I}_n & \dots & \mu_{mm}\mathcal{I}_n \end{pmatrix}, \quad (97)$$

Let us apply the Wigner theorem for splitting the linearized system $\ddot{\vec{\delta}} = \mathcal{J}(t)\vec{\delta}$ near the dynamical regime (a bush of modes) with symmetry group G . To this end, we will assume that \mathcal{H} and Γ of the theorem are respectively the Jacobi matrix $\mathcal{J}(t)$ and the natural representation of the group G .

To implement this splitting explicitly we must pass from the old basis $\vec{\Phi}_{old} = \{\vec{e}_1, \vec{e}_2, \dots, \vec{e}_N\}$ of the natural space to the new basis $\vec{\Phi}_{new} = \{\vec{\varphi}_1, \vec{\varphi}_2, \dots, \vec{\varphi}_N\}$ formed by the complete set of the basis vectors $\vec{\varphi}_k$ ($k = 1, 2, \dots, N$) of all the irreps of the group G . If $\vec{\Phi}_{new} = \mathcal{S}\vec{\Phi}_{old}$, then the unitary transformation

$$\mathcal{J}_{new}(t) = \mathcal{S}^\dagger \mathcal{J}_{old} \mathcal{S} \quad (98)$$

produces the above-discussed block-diagonal matrix $\mathcal{J}_{new}(t)$ of the linearized system $\ddot{\vec{\delta}}_{new} = \mathcal{J}_{new}(t)\vec{\delta}_{new}$ (here $\vec{\delta}_{old} = \mathcal{S}\vec{\delta}_{new}$).

3.6.3. Splitting schemes

The above-discussed implicit decomposition of the Jacobi matrix $\mathcal{J}(t)$ is a cumbersome procedure and, therefore, it is interesting to know beforehand to what extent it can be useful in specific cases. This can be easily determined by means of the theory of *characters* of group representations.

Let us consider such an approach by determining the *splitting scheme* of the linearized system $\ddot{\vec{\delta}} = \mathcal{J}(t)\vec{\delta}$. In other words, we would like to find out how many subsystems of different dimensions can be obtained as a result of the decomposition of the Jacobi matrix.

Each block \mathcal{D}_j in the decomposition (96) of the matrix $\mathcal{H} \equiv \mathcal{J}(t)$ generates an independent subsystem of $n_j m_j$ equations of the linearized system. However, each subsystem automatically splits into n_j new subsystems consisting of m_j differential equations, as a consequence of the specific structure of these blocks [see Eq. (97)]. For example, if a certain block for the matrix $\mathcal{J}(t)$ possesses the form ($n_j = 3$, $m_j = 2$)

$$\mathcal{J}_j(t) = \begin{pmatrix} \mu_{11}\mathcal{I}_3 & \mu_{12}\mathcal{I}_3 \\ \mu_{21}\mathcal{I}_3 & \mu_{22}\mathcal{I}_3 \end{pmatrix},$$

it is easy to check that one can obtain from the system $\ddot{\vec{\delta}} = \mathcal{J}(t)\vec{\delta}$ three independent 2×2 subsystems with one and the same matrix

$$\mathcal{M} = \begin{pmatrix} \mu_{11} & \mu_{12} \\ \mu_{21} & \mu_{22} \end{pmatrix}.$$

Thus, to obtain the splitting scheme of the linearized system $\ddot{\vec{\delta}} = \mathcal{J}\vec{\delta}$, for each irrep Γ_j of the bush symmetry group G , one must find two numbers— n_j (the dimension of Γ_j) and m_j (the subduction frequency from Eq. (95)).

The multiplicity numbers m_j can be found by means of Eq. (A.13) of Appendix A in terms of the characters $\chi_j(g)$ of the irreps Γ_j , which are well-known for many groups of discrete symmetry (in particular the point symmetry groups) and $\chi_\Gamma(g)$, which represents the character of the reducible representation Γ . These characters can be determined without the explicit construction of the matrices of the natural representation Γ .

A quick and simple method for obtaining $\chi_\Gamma(g)$ can be found in many textbooks (see, for example, [Landau & Lifshitz, 1977]) in connection with studying the small vibrations of multiatomic molecules. The main point of the method is that, for a fixed $g \in G$, the only atoms that contribute to $\chi_\Gamma(g)$ are those whose position does not change under the action of g on the molecule. Moreover, this contribution is determined by the trace of the three-dimensional matrix associated with the symmetry element g . For example, the contribution to $\chi_\Gamma(g)$ from any atom invariant under the action of a rotation by an angle φ is $1 + 2\cos(\varphi)$, while that for a mirror rotation is $-1 + 2\cos(\varphi)$.

Let us illustrate this in the case of an N -particle monoatomic chain for $N \gg 1$. We denote by $B[\hat{a}^m, \dots]$ the bush $B[G]$, with the symmetry group G containing the translational subgroup $[\hat{a}^m]$ and dots standing for other generators of the group G . In [Chechin & Zhukov, 2006], the following theorem was proved:

Theorem 3. *The linear stability analysis of any bush $B[\hat{a}^m, \dots]$ in an N -degrees-of-freedom monoatomic chain can be reduced to the stability analysis of isolated subsystems of the second order differential equations with time-dependent coefficients whose dimension does not exceed the integer number m .*

Corollary. If the bush dimension is d , one can perform the above analysis for subsystems of *autonomous* differential equations with dimensions not exceeding $(m + d)$.

For example, the scheme for the linearized system about a one-dimensional bush $B[\hat{a}^3, \hat{i}]$ of an arbitrary nonlinear chain with $N = 12$ particles allows us to split the 12 linearized equations into two one-dimensional, two two-dimensional and two three-dimensional subsystems, which are all independent from each other.

3.6.4. Stability diagrams for NNMs in the FPU chains

The above discussed decomposition of the full linearized system $\ddot{\vec{\delta}} = \mathcal{J}(t)\vec{\delta}$ into independent subsystems of small dimension permits one to analyze efficiently the stability of a given bush in monoatomic chains with arbitrarily large number of particles. Using this idea, the stability diagrams for all the one-dimensional bushes (NNMs) in both FPU- α and FPU- β chains were obtained in [Chechin *et al.*, 2005]. As an example, we reproduce here in Fig. 6 the stability diagram for the bush $B[\hat{a}^4, \hat{i}u]$ of the FPU- β chain.

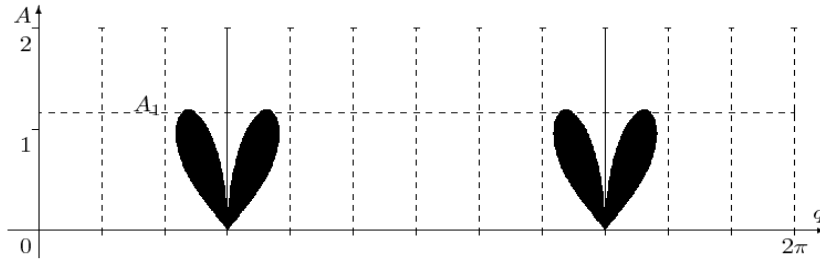


Fig. 6. Regions of stability (white color) of different modes of the FPU- β chain, interacting parametrically with the one-dimensional bush $B[a^4, iu]$.

In this diagram, each point (A, q) provides a value of the bush mode amplitude A and the wave number $q = \frac{2\pi j}{N}$ associated with the index j of a particular mode. The black points (A, q) correspond to the case where the mode $j = q \frac{N}{2\pi}$ becomes excited because of its parametric interaction with the mode of the bush $B[\hat{a}^4, \hat{i}u]$. The white color denotes the opposite case: the corresponding mode j is zero initially and continues to be zero in spite of its interaction with the considered bush. Such diagrams allow one to study stability of one-dimensional bushes not only for finite N , but also for the case $N \rightarrow \infty$ (for more details see [Chechin *et al.*, 2005]).

In the particular diagram depicted in Fig. 6, we denote the permissible values of the wave number q for $N = 12$ by the dotted vertical lines ($q = 2\pi j/12, j = 1, 2, \dots, 12$). The black color corresponds to the regions of unstable motion in the plane $(q - A)$. From Fig. 6 one can see that, for an FPU- β chain with $N = 12$ particles, the NNM $B[a^4, iu]$ with $\vec{c} = \{1, -1, -1, 1 \mid 1, -1, -1, 1 \mid 1, -1, -1, 1\}$ is *stable* for *every* amplitude $A > 0$ (at least up to $A = 20$), since the vertical dotted lines do not cross the rabbit-ear shaped black (unstable) regions. In fact, the mode $B[a^4, iu]$ is also stable for chains with $N = 4$ and $N = 8$ particles, since the corresponding vertical dotted lines are *even more distant* from each other than for $N = 12$.

In the case $N = 16$, however, there exist dotted vertical lines which are *tangent* to the rabbit-ear unstable regions, while for $N > 16$ (note that $N \bmod 4 = 0$ must hold!) these lines begin to *cross* the unstable regions. Therefore, we can conclude that the considered nonlinear normal mode in FPU- β chains with $N > 16$ becomes unstable for amplitude values, which lie within the black regions in Fig. 6. The case $N = 16$ represents the “boundary” between stable and unstable behavior of the $B[a^4, iu]$ NNM.

Using Fig. 6, one can verify that the *critical* amplitude A_c of the nonlinear normal mode $B[a^4, iu]$, at which stability is lost, decreases with increasing N . Thus, one can evaluate numerically the corresponding

scaling law of the function $A_c(N)$ in the thermodynamic limit, where $N \rightarrow \infty$ and $E \rightarrow \infty$ with E/N fixed [Chechin & Ryabov, 2010]. It is also interesting to note that if the amplitude of the NNM $B[\hat{a}^4, \hat{i}\hat{u}]$ exceeds a certain critical value $A^* \approx 1.19$ (see Fig. 6), this NNM becomes stable again! Indeed, for $A > A^*$, the horizontal lines of $A = \text{constant}$ do not intersect any unstable regions.

Let us summarize the results reviewed of this section concerning the stability of bushes of NNMs:

(a) If the amplitude of a given NNM (one-dimensional bush) exceeds a certain limit, this mode can lose its stability because of specific interactions with some other NNMs of the considered system. As a result, the symmetry of the vibrational state becomes lower and the system passes to the dynamical regime of a higher dimensional bush whose dimension $n > 1$. This means that the *periodic motion* of the considered NNM becomes *quasiperiodic* with $n > 1$ basic frequencies, which are rationally independent.

(b) Of course, one cannot use Floquet theory to study stability of bushes whose dimension $n > 1$, but the group theoretical method presented in subsection III.F can simplify significantly the analysis. Indeed, the methods we have described allow us to split the linearized equations of motion near a bush into a number of independent subsystems whose dimension can be much smaller than that of the full system. Thus, when a given bush loses its stability and transforms into another one of higher dimension, one may ask: What new modes turn out to be involved into the corresponding vibrational process?

The following questions also arise: How can one determine the dimension n of these quasiperiodic orbits and the frequencies of the corresponding tori? What are the properties of the dynamics in their vicinity? How can the stability (and hence the existence) of these tori be determined accurately and efficiently so as to gain a more global picture of the stability of motion of the system? To answer these questions, we need to examine the phenomena of energy localization and NNM interaction on low-dimensional tori, employing analytical methods as well as the numerical approach of the Generalized Alignment Indices (GALI), as we describe in Section IV below.

4. Energy localization on q -tori and stability of motion in FPU chains

In sections I–III of this paper, we discussed extensively a group theoretical method by which one can construct exact solutions of mechanical systems described by N -degree of freedom Hamiltonians. In particular, using as an example the FPU N -particle chains, under periodic boundary conditions, we exploited symmetry groups of their equations of motion to determine all continuations of linear normal modes (termed here nonlinear normal modes or NNMs), which constitute the so-called one-dimensional bushes. Next, we considered linear combinations of these NNMs, in ways which do not excite other modes and were able to construct higher ($s > 1$)-dimensional bushes, which at low enough energies are *quasiperiodic*, possessing n generally incommensurate frequencies.

In this section, we complete our review by describing two more recent developments in the study of low-dimensional tori of the FPU system, in which one of us and his co-workers have played a crucial role [Skokos *et al.*, 2008, 2007; Bountis *et al.*, 2008; Christodoulidi *et al.*, 2010]: The first one starts, as in the earlier sections, with the construction of $s(> 1)$ -dimensional bushes by linear combinations of NNMs of *low wave numbers* $q = 1, 2, 3, \dots$ and establishes the important property of *exponential localization* of the energies of the Fourier modes belonging to the so-called q -tori, through which the well-known paradox of FPU recurrences can be better understood [Bountis *et al.*, 2008; Christodoulidi *et al.*, 2010]. It is important to emphasize that this approach does not depend on the symmetries of the system or the type of boundary conditions.

The second development concerns a more *comprehensive method* for studying the stability of quasiperiodic orbits, without resorting to Floquet analysis, but using instead the recently introduced spectrum of GALI indicators [Skokos *et al.*, 2008, 2007]. Indeed, the GALI's asymptotic behavior as $t \rightarrow \infty$ (typically up to $t = 10^6 - 10^8$): (i) determines the *dimension* s of the torus, if the GALI_k indices tend to a constant for $k = 2, 3, \dots, s$ (and decay by algebraic power laws for $s < k \leq 2N$) and (b) predicts the *instability* of a torus beyond an energy threshold E_{th} if, for $E > E_{th}$, *all* GALI_k start, at some time t , to *decay exponentially*, indicating that the orbit we are following is *not quasiperiodic* but diffuses chaotically away from a torus that at energies $E \geq E_{th}$ no longer exists.

4.1. Energy localization on q -tori and FPU recurrences

We shall use as our main example the FPU Hamiltonian for a chain of N particles, (99), which we rewrite here for convenience:

$$H = \frac{1}{2} \sum_{k=1}^N p_k^2 + \frac{1}{2} \sum_{k=0}^N (x_{k+1} - x_k)^2 + \frac{\alpha}{3} \sum_{k=0}^N (x_{k+1} - x_k)^3 + \frac{\beta}{4} \sum_{k=0}^N (x_{k+1} - x_k)^4 \quad (99)$$

We shall discuss primarily f.b.c., setting $x_0 = x_{N+1} = 0$, since the case of p.b.c. does not present any major differences.

For the FPU β -model ($\alpha = 0$) of this mechanical system the normal mode canonical variables (Q_q, P_q) are introduced by the canonical transformations

$$x_k = \sqrt{\frac{2}{N+1}} \sum_{q=1}^N Q_q \sin\left(\frac{qk\pi}{N+1}\right), \quad p_k = \sqrt{\frac{2}{N+1}} \sum_{q=1}^N P_q \sin\left(\frac{qk\pi}{N+1}\right) \quad (100)$$

Substitution of (100) into (99) brings the Hamiltonian (99) in the form $H = H_2 + H_4$, where the quadratic part represents N uncoupled harmonic oscillators

$$H_2 = \sum_{q=1}^N \frac{P_q^2 + \Omega_q^2 Q_q^2}{2} \quad (101)$$

with normal mode frequencies

$$\Omega_q = 2 \sin\left(\frac{q\pi}{2(N+1)}\right), \quad 1 \leq q \leq N \quad (102)$$

On the other hand, the quartic part of the Hamiltonian becomes

$$H_4 = \frac{\beta}{2(N+1)} \sum_{q,l,m,n=1}^N C_{q,l,m,n} \Omega_q \Omega_l \Omega_m \Omega_n Q_q Q_l Q_m Q_n \quad (103)$$

where the coefficients $C_{q,l,m,n}$ are non-zero only for particular combinations of the indices q, l, m, n , i.e.

$$C_{q,l,m,n} = \begin{cases} 1 & \text{if } q \pm l \pm m \pm n = 0 \\ -1 & \text{if } q \pm l \pm m \pm n = \pm 2(N+1) \end{cases} \quad (104)$$

with all possible choices of the \pm signs taken into account. Thus, in the new variables, the equations of motion are expressed as follows:

$$\ddot{Q}_q + \Omega_q^2 Q_q = -\frac{\beta}{2(N+1)} \sum_{l,m,n=1}^N C_{q,l,m,n} \Omega_q \Omega_l \Omega_m \Omega_n Q_l Q_m Q_n \quad (105)$$

The question we wish to pursue here is what happens to the (linear) normal modes

$$E_q = (P_q^2 + \Omega_q^2 Q_q^2)/2, \quad q = 1, 2, \dots, N \quad (106)$$

when $\beta \neq 0$? In other words, if we choose initial conditions $x_k = x_k(0)$, $p_k = p_k(0)$, $k = 1, 2, \dots, N$ in (100) such that a small number (one, two, or more) modes (106) are excited, with energies E_q , $q = 1, 2, \dots$, will these modes retain the total energy E (and only exchange it among themselves), or will they share it equally with all other modes, as statistical mechanics of ergodic systems would require?

This was precisely the question asked by Fermi, Pasta and Ulam in their famous experiments of the early 1950's [Fermi *et al.*, 1955]. As is well-known, they obtained the surprising result that, at small E values, energy was *not shared* among all modes, but kept returning to the initially excited ones, giving rise to the so-called FPU recurrences. There have been hundreds of papers to date analyzing this phenomenon (for a recent review see [Berman & Izrailev, 2005]) and we shall also provide our own explanation here, using the concept of q -tori [Christodoulidi *et al.*, 2010]. The difference between q -tori and the multidimensional

bushes discussed in earlier sections is that the set of NNMs excited in a bush does not change in time, while in q -tori all modes (106) are active in general, albeit with exponentially decreasing energies.

We now recall the theorem by Lyapunov [Lyapunov, 1892] mentioned in the Introduction, which states that if the frequencies Ω_q of the *linear* normal modes (102) of an N -degree-of-freedom Hamiltonian system are incommensurate, these modes survive for $\beta \neq 0$. This condition of non-commensurability is indeed satisfied in the f.b.c. case (102) for many N , e.g. a power of two minus 1, or a prime number minus 1, among others [Hemmer, 1959]. It fails, however, in the p.b.c. case, for which the frequency spectrum given by

$$\Omega_q = 2 \sin\left(\frac{q\pi}{N}\right), \quad 1 \leq q \leq N \quad . \quad (107)$$

is commensurate *for every* N , since $\sin(q\pi/N) = \sin((N-q)\pi/N)$, for $q = 1, 2, \dots, [N/2]$. Thus, the arguments and methods based on discrete symmetry groups, which we presented in section II, turn out to be extremely useful for proving the existence of NNMs in the p.b.c. case.

The group theoretical approach considers orbits as dynamical states, see Eq. (7), consisting of patterns (extended primitive cells) which are periodically repeated, see e.g. (14)–(20), (30). By construction, therefore, these states are built by modes that correspond to high wavenumbers $q = N/2, 3N/4, \dots$, etc., while their symmetries may be expressed by N -dimensional vectors of the type shown in (67). Indeed, these vectors provide an orthonormal basis, by which one can construct multi-dimensional bushes using linear combinations of such NNMs, as described in subsection III.D.

There is, however, a more direct way to construct quasiperiodic orbits, which neither employs symmetries nor uses special q -values to achieve this purpose: It is the well-known Poincaré–Linstedt method, which starts with any number of modes with incommensurate frequencies ω_{q_i} , for $i = 1, 2, \dots, n$, and approximates the orbits through the solutions of the linear problem, $x_i(t) = A_i \cos(\omega_{q_i} t)$. Then, through interactions provided by the nonlinear terms of the equations of motion, new q -modes are born, which, interestingly enough, have exponentially decaying energies in the E_q vs. q space. These so-called q -tori are seen to be n -dimensional (with n as low as 2 or 3), depending on how many modes are initially excited and are *stable* in the sense that the tangent space of the corresponding quasiperiodic orbits is spanned by n linearly independent vectors, at least for very long times and sufficiently low energies.

Let us see how all this is done explicitly on an example of the FPU- β model (99) with f.b.c. and $N = 8$: We shall construct a 2-dimensional torus representing the continuation of the $q_1 = 1$ and $q_2 = 2$ linear normal modes, $Q_1(t) = A_1 \cos \Omega_1 t$, $Q_2 = A_2 \cos \Omega_2 t$, for $\beta \neq 0$ and special values of A_1, A_2 . Following the Poincaré - Lindstedt approach, we seek solutions $Q_q(t)$, $q = 1, \dots, 8$ expanded as series in the parameter $\sigma = \beta/2(N+1)$, namely

$$Q_q(t) = Q_q^{(0)}(t) + \sigma Q_q^{(1)}(t) + \sigma^2 Q_q^{(2)}(t) + \dots, \quad q = 1, \dots, 8 \quad . \quad (108)$$

For the motion to be quasi-periodic on a two-torus, the functions $Q_q^{(r)}(t)$ must, at any order r , be trigonometric polynomials involving only two frequencies ω_1 and ω_2 (and their multiples). Moreover, these must arise as small corrections of the linear normal mode frequencies Ω_1, Ω_2 , given by series expansions in powers of σ , as:

$$\omega_q = \Omega_q + \sigma \omega_q^{(1)} + \sigma^2 \omega_q^{(2)} + \dots \quad q = 1, 2 \quad . \quad (109)$$

As is well-known, the $\omega_q^{(i)}$, $i = 1, 2, \dots$ in (108) are determined by the requirement that no secular terms (of the type $t \sin \omega_q t$ etc.) arise in the equations of motion.

For example, the equation for the first mode, contains on its right hand side (r.h.s) terms of the form:

$$\ddot{Q}_1 + \Omega_1^2 Q_1 = -\sigma(3\Omega_1^4 Q_1^3 + 6\Omega_1^2 \Omega_2^2 Q_1 Q_2^2 + 3\Omega_1^3 \Omega_3 Q_1^2 Q_3 + \dots) \quad (110)$$

Substituting Ω_1 on the l.h.s. of Eq.(110) by the expression obtained by squaring (109) and solving for Ω_1^2 , inserting the expansions (108) into (110) and grouping together terms of the same order, we find that at zeroth order $\ddot{Q}_1^{(0)} + \omega_1^2 Q_1^{(0)} = 0$, while at first order the following equation is satisfied

$$\begin{aligned} \ddot{Q}_1^{(1)} + \omega_1^2 Q_1^{(1)} = & 2\Omega_1 \omega_1^{(1)} Q_1^{(0)} - 3\Omega_1^4 (Q_1^{(0)})^3 - 6\Omega_1^2 \Omega_2^2 Q_1^{(0)} (Q_2^{(0)})^2 \\ & - 3\Omega_1^3 \Omega_3 (Q_1^{(0)})^2 Q_3^{(0)} + \dots \end{aligned} \quad (111)$$

Repeating the above procedure for modes 2 and 3, we find that their zeroth order equations also take the harmonic oscillator form, i.e. we have:

$$\ddot{Q}_i^{(0)} + \omega_i^2 Q_i^{(0)} = 0, \quad i = 1, 2 \quad \ddot{Q}_3^{(0)} + \Omega_3^2 Q_3^{(0)} = 0 \quad . \quad (112)$$

Note that the *corrected* frequencies ω_1, ω_2 appear in the zeroth order equations for the modes 1 and 2, while the *uncorrected* frequency Ω_3 appears in the zeroth order equation of the mode 3 (similarly, $\Omega_4, \dots, \Omega_8$ appear in the zeroth order equations of the modes $q = 4, \dots, 8$). We now proceed with the solutions of (112) (with zero velocities at $t = 0$) which read:

$$Q_1^{(0)}(t) = A_1 \cos \omega_1 t, \quad Q_2^{(0)}(t) = A_2 \cos \omega_2 t, \quad Q_3^{(0)}(t) = A_3 \cos \Omega_3 t$$

where the amplitudes A_1, A_2, A_3 are arbitrary. If the orbit is to lie on a two-torus with frequencies ω_1 and ω_2 only, we must set $A_3 = 0$. In the same way, the zeroth order equations $\ddot{Q}_q^{(0)} + \Omega_q^2 Q_q^{(0)} = 0$, for the remaining modes $q = 4, \dots, 8$, would yield solutions with new frequencies and hence we need to set $A_4 = A_5 = \dots = A_8 = 0$ also. Thus, we are left with only two non-zero free amplitudes to determine: A_1, A_2 .

As we explain in detail in [Christodoulidi *et al.*, 2010], equation (111) can be simplified dramatically and upon substitution of $Q_1^{(0)}(t) = A_1 \cos \omega_1 t$, $Q_2^{(0)}(t) = A_2 \cos \omega_2 t$ reduces to:

$$\begin{aligned} \ddot{Q}_1^{(1)} + \omega_1^2 Q_1^{(1)} &= 2\Omega_1 \omega_1^{(1)} A_1 \cos \omega_1 t - 3\Omega_1^4 A_1^3 \cos^3 \omega_1 t \\ &\quad - 6\Omega_1^2 \Omega_2^2 A_1 A_2^2 \cos \omega_1 t \cos^2 \omega_2 t \quad . \end{aligned} \quad (113)$$

We now fix $\omega_1^{(1)}$ so that no secular terms appear in the solution, yielding

$$\omega_1^{(1)} = \frac{9}{8} A_1^2 \Omega_1^3 + \frac{3}{2} A_2^2 \Omega_1 \Omega_2^2$$

while we also determine $Q_1^{(1)}$ as:

$$\begin{aligned} Q_1^{(1)}(t) &= \frac{3A_1^3 \Omega_1^4 \cos 3\omega_1 t}{32\omega_1^2} + \frac{3A_1 A_2^2 \Omega_1^2 \Omega_2^2 \cos(\omega_1 + 2\omega_2)t}{2[(\omega_1 + 2\omega_2)^2 - \omega_1^2]} \\ &\quad + \frac{3A_1 A_2^2 \Omega_1^2 \Omega_2^2 \cos(\omega_1 - 2\omega_2)t}{2[(\omega_1 - 2\omega_2)^2 - \omega_1^2]} \quad . \end{aligned} \quad (114)$$

Repeating the above analysis for the second mode, $Q_2(t)$, we obtain the frequency correction of the second mode:

$$\omega_2^{(1)} = \frac{9}{8} A_2^2 \Omega_2^3 + \frac{3}{2} A_1^2 \Omega_1^2 \Omega_2$$

and the first order solution

$$\begin{aligned} Q_2^{(1)}(t) &= \frac{3A_2^3 \Omega_2^4 \cos 3\omega_2 t}{32\omega_2^2} + \frac{3A_1^2 A_2 \Omega_1^2 \Omega_2^2 \cos(2\omega_1 + \omega_2)t}{2[(2\omega_1 + \omega_2)^2 - \omega_2^2]} \\ &\quad + \frac{3A_1^2 A_2 \Omega_1^2 \Omega_2^2 \cos(2\omega_1 - \omega_2)t}{2[(2\omega_1 - \omega_2)^2 - \omega_2^2]} \end{aligned} \quad (115)$$

which has a similar structure as the first order solution of the first mode. For the third order term there is no frequency correction, and we find

$$\begin{aligned} Q_3^{(1)}(t) &= \frac{A_1^3 \Omega_1^3 \Omega_3}{4} \left(\frac{3 \cos \omega_1 t}{\omega_1^2 - \Omega_3^2} + \frac{\cos 3\omega_1 t}{9\omega_1^2 - \Omega_3^2} \right) \\ &\quad + \frac{3A_1 A_2^2 \Omega_1 \Omega_2^2 \Omega_3}{4} \left(\frac{\cos(\omega_1 - 2\omega_2)t}{(\omega_1 - 2\omega_2)^2 - \Omega_3^2} + \frac{\cos(\omega_1 + 2\omega_2)t}{(\omega_1 + 2\omega_2)^2 - \Omega_3^2} + \frac{2 \cos \omega_1 t}{\omega_1^2 - \Omega_3^2} \right) \quad . \end{aligned} \quad (116)$$

We thus proceed up to the sixth mode and find that all the functions $Q_3^{(0)}, \dots, Q_6^{(0)}$ are equal to zero, while the functions $Q_3^{(1)}, \dots, Q_6^{(1)}$ are non zero. However, a new situation appears when we arrive at the seventh

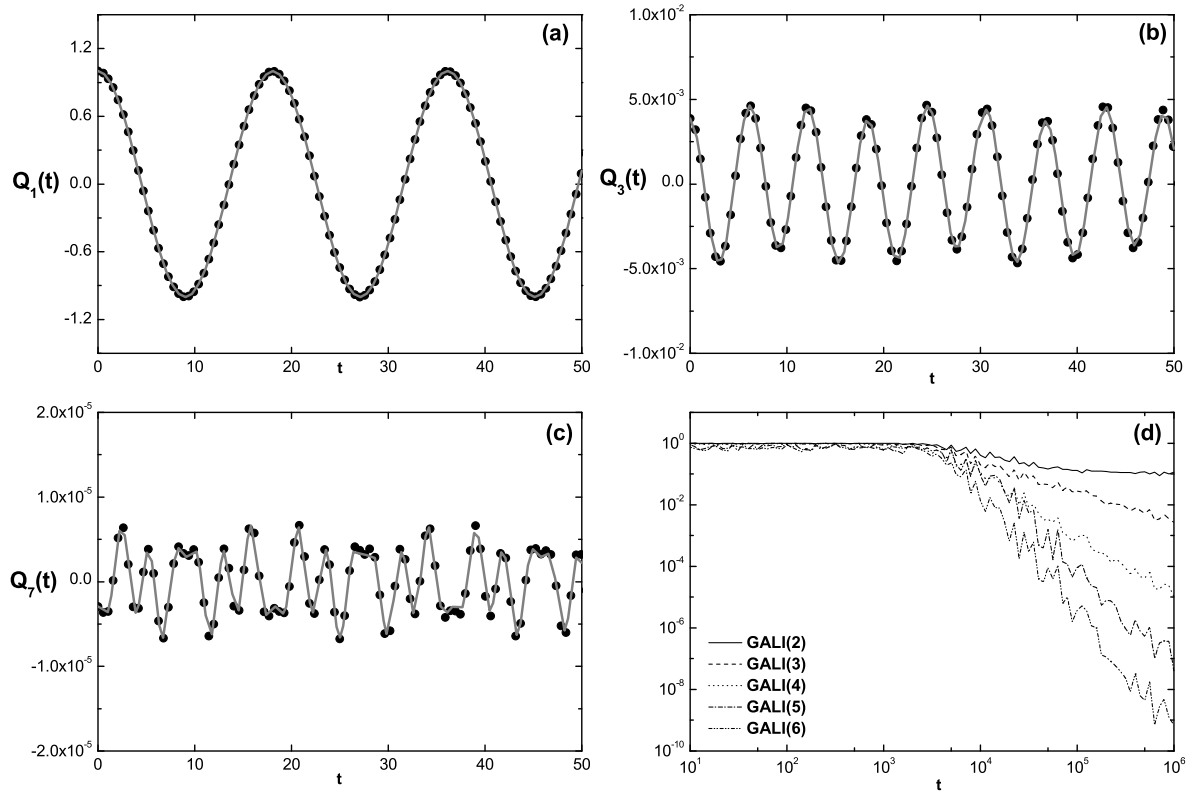


Fig. 7. Comparison of numerical (points) versus analytical (solid line) solutions, using the Poincaré - Lindstedt series up to order $O(\sigma^2)$, for the temporal evolution of the modes (a) $q = 1$, (b) $q = 3$, (c) $q = 7$, when $A_1 = 1$, $A_2 = 0.5$, and $N = 8$, $\beta = 0.1$ and (d) the time evolution of the indices GALI₂ to GALI₆ up to a time $t = 10^6$ show that the motion lies on a 2-dimensional torus.

and eighth modes. A careful inspection of the equation for $Q_7^{(1)}(t)$ shows that there can be *no term* on the r.h.s. which does not involve some of the functions $Q_3^{(0)}, \dots, Q_8^{(0)}$, according to the selection rules for the coefficients of Eq.(104). Since all these functions are zero, we must set $Q_7^{(1)}(t) = 0$, so as not to introduce a *third* frequency in the solutions, whence the series expansion (108) for $Q_7(t)$ necessarily starts with terms of order at least $O(\sigma^2)$. The same holds true for the equation determining $Q_8^{(1)}(t)$.

In [Christodoulidi *et al.*, 2010] it is shown that the Poincaré-Linstedt scheme is *consistent*, in the sense that the series constructed above will *never* encounter terms with zero denominator, as long as our parameters lie in the complement of a Cantor set in the ω_1, ω_2 (or A_1, A_2) space. We then discuss the question of *convergence* of the series, which is in general a very difficult issue. However, as we also explain below, the fact that the amplitudes squared (or, equivalently the energies) of the higher order terms of our series are seen to decrease *exponentially* with q suggests that our series may indeed be absolutely convergent, after all.

To verify this numerically, let us use the analytical solutions (108) at $t = 0$ as initial conditions to integrate the equations of motion and compare the computed $Q_i(t)$, $i = 1, 3, 7$ with our analytical formulas. We also apply the GALI criterion (see subsection IV.B) to show that the solutions lie indeed on two-dimensional tori. As shown in Figures 7a-c, the numerically evaluated $Q_1(t)$, $Q_3(t)$ and $Q_7(t)$ are in excellent agreement with the analytical solution truncated at second order with respect to σ , when $N = 8$, $\beta = 0.1$, and $A_1 = 1$, $A_2 = 0.5$.

Concerning Fig. 7d, let us note that, if an orbit lies on a *stable* s -dimensional torus, the indicators GALI₂, ..., GALI_s, discussed in the next subsection, are nearly *constant*, oscillating about *non-zero* values, while the GALI_{s+j}, $j = 1, 2, \dots, 2N - s$ decay asymptotically by power laws, as t^{-j} [Skokos *et al.*, 2007,

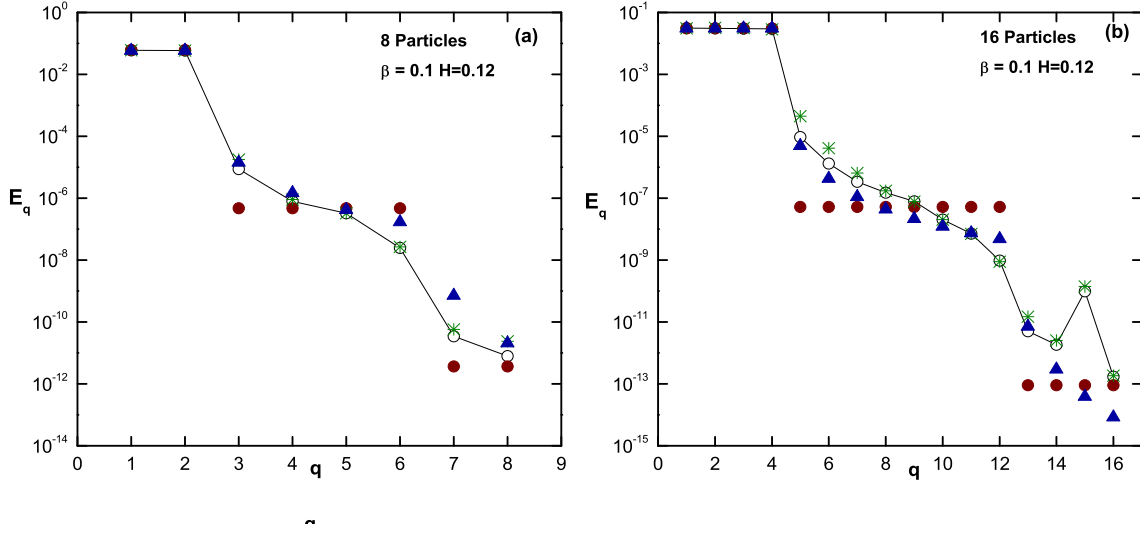


Fig. 8. The average harmonic energy E_q of the q -th mode as a function of q , after a time $T = 10^6$ for (a) the 2-torus of Fig.7a and (b) a 4-torus solution (open circles). The stars are E_q values calculated via the analytical representation of the solutions $Q_q(t)$ by the Poincaré-Lindstedt series. The filled circles show a theoretical estimate based on the average energy of suitably defined groups of modes (see Eq.(120) and relevant discussion in the text).

2008; Bountis *et al.*, 2008].

This is precisely what we observe in Fig. 7d. Namely, the GALI_2 index stabilizes at a constant value $\text{GALI}_2 \simeq 0.1$, while all subsequent indices, starting from GALI_3 decay following a power law as predicted by the theory. Thus, we conclude that the motion lies on a 2-torus, exactly as suggested by the Poincaré-Lindstedt construction, despite the fact that some excitation was provided initially to all modes. In fact, we have carried out many such experiments, starting initially with $s > 2$ modes and, in every case, the analytical solutions were found to be very accurate, while all the GALI indicators showed that they lie on s -dimensional tori.

Let us now evaluate, for such excitations, the average harmonic energy E_q of the q mode and plot it as a function of the wavenumber q , after a time interval $T = 10^6$. As we observe in Fig. 8a,b, the numerical results shown by the white circles are very close to the analytical ones represented by the stars, for an initial excitation with $s = 2$ and one with $s = 4$ modes respectively. Furthermore, what is clearly evident in these semi-log plots, is that the magnitude of the E_q falls exponentially, though not with one and the same exponent. Let us examine more closely this phenomenon of *energy localization*:

The average size of the oscillation amplitudes of each mode on an s -dimensional q -torus follows from norm estimates of all terms of the form $Q_{q^{(k)}}^{(k)}(t)$ appearing in equations such as Eq.(114), where $q^{(k)}$ denotes the indices of all modes excited at order k of the perturbation. If we define by $A^{(k)}$ the mean value of all the norms $\|Q_{q^{(k)}}\|$, we obtain the estimate:

$$A^{(k)} = \frac{(Cs)^k A_0^{2k+1}}{2k+1} \quad (117)$$

where $A_0 \equiv A^{(0)}$ is the mean amplitude of the oscillations of all modes excited at the zeroth order of the theory, and C is a constant of order $O(1)$. The proof of (117) is provided in [Christodoulidi *et al.*, 2010], Appendix B, in which the analytical estimate $C \simeq 3/2$ was given. In fact, (117) is a generalization of the estimate given by Flach *et al.* [Flach *et al.*, 2005, 2006] for q -breathers, while the two estimates become identical (except for the precise value of C) if one sets $s = 1$ in Eq.(117), and $q_0 = 1$ in Flach's q -breather formula.

Note, of course, that, with $|CsA_0^2| < 1$, Eq. (117) clearly implies that the amplitudes (and corresponding energies) of the modes of these s -dimensional tori are decreasing exponentially with k . This is reminiscent of the localization properties of q -breathers, studied by Flach *et al.* [Flach *et al.*, 2005, 2006] in connection

with the paradox of FPU recurrences. We, therefore, decided to call all s -dimensional tori whose modes are exponentially localized q -tori.

In fact, these s -dimensional q -tori, when excited at high enough energies, give rise to the so-called “natural packets” of $m > s$ modes, which cause the breakdown of FPU recurrences by becoming resonant, as suggested in a number of papers (see e.g. [Berchiolla *et al.*, 2004], [Luca *et al.*, 1999]) on the FPU β -chain. Thus, q -tori offer a “bridge” between the scenario described in these references and the arguments based on energy localization of q-breathers to provide a more complete interpretation of the FPU recurrences.

Furthermore, using (117), it is possible to obtain ‘piecewise’ estimates of the energy of each group, using a formula for the average harmonic energies $E^{(k)}$ of the modes $q^{(k)}$. To see how this is done, note that the total energy E given to the system can be estimated as the sum of the energies of the modes $1, \dots, s$ (the remaining modes yield only small corrections to the total energy), as

$$E \sim s\omega_{q^{(0)}}^2 A_0^2 \sim \frac{\pi^2 s^3 A_0^2}{(N+1)^2}.$$

On the other hand, the energy of each mode $q^{(k)}$ can be estimated from

$$E^{(k)} \sim \frac{1}{2} \Omega_{q^{(k)}}^2 \left(\frac{\beta}{2(N+1)} \right)^{2k} (A^{(k)})^2 \sim \frac{\pi^2 s^2 (Cs\beta)^{2k} A_0^{4k+2}}{2^{2k+1} (N+1)^{2k+2}}$$

which, in terms of the total energy E , yields

$$E^{(k)} \sim \frac{E}{s} \left(\frac{C^2 \beta^2 (N+1)^2 E^2}{\pi^4 s^4} \right)^k. \quad (118)$$

Eq.(118) is very similar to the corresponding equation for q-breathers [Flach *et al.*, 2006]

$$E_{(2k+1)q_0} \sim E_{q_0} \left(\frac{9\beta^2 (N+1)^2 E^2}{64\pi^4 q_0^4} \right)^k \quad (119)$$

where q_0 is the unique mode excited at zeroth order of the perturbation theory and the integer s plays in Eq.(118) a role similar to that of q_0 in Eq.(119). This means that the energy profile of a q-breather with $q_0 = s$ obeys the same exponential law as the energy profile of the s -dimensional q-torus.

Still, the most important feature of the solutions on q -tori is that their profile remains *invariant* as N increases, provided that: i) a *constant fraction* $M = s/N$ of the spectrum is initially excited, (i.e. that s increases proportionally with N), and ii) the *specific energy* $\varepsilon = E/N$ *remains constant*. Thus, in terms of the specific energy ε , (118) takes the form

$$E^{(k)} \sim \frac{\varepsilon}{M} \left(\frac{C^2 \beta^2 \varepsilon^2}{\pi^4 M^4} \right)^k \quad (120)$$

i.e. the profile becomes *independent* of N . A similar behavior is recovered in the q-breather solutions provided that the ‘seed’ mode q_0 varies linearly with N , as was shown in detail in refs.[Flach *et al.*, 2007; Kanakov *et al.*, 2007].

The ‘stepwise’ profiles predicted by Eq.(118) in the case of exact q-tori solutions are shown by filled circles in Fig. 8, concerning examples of a 2-torus (see Fig. 7a) and a 4-torus solution (in all fittings we set $C = 1$ for simplicity). From these we see that the theoretical ‘piecewise’ profiles yield nearly the same “plateaus” and average exponential slope of the profiles obtained numerically, or analytically by the Poincaré - Lindstedt method.

Naturally, regarding the relevance of the q-tori solutions for the interpretation of FPU recurrences, one must verify whether Eqs.(118) or (120) retain their predictive power in the case of generic FPU trajectories which, by definition, are started close to, but not exactly on a q-torus.

To answer this question let us examine the results presented in Figures 9 and 10. Figure 9 shows the energy localization profile in numerical experiments in which β is kept fixed ($\beta = 0.3$), while N takes the values $N = 64$, $N = 128$ and $N = 256$. In all six panels of Fig. 9 the FPU-trajectories are computed starting with initial conditions in which *only* the $s = 4$ (for $N = 64$), $s = 8$ (for $N = 128$) and $s = 16$

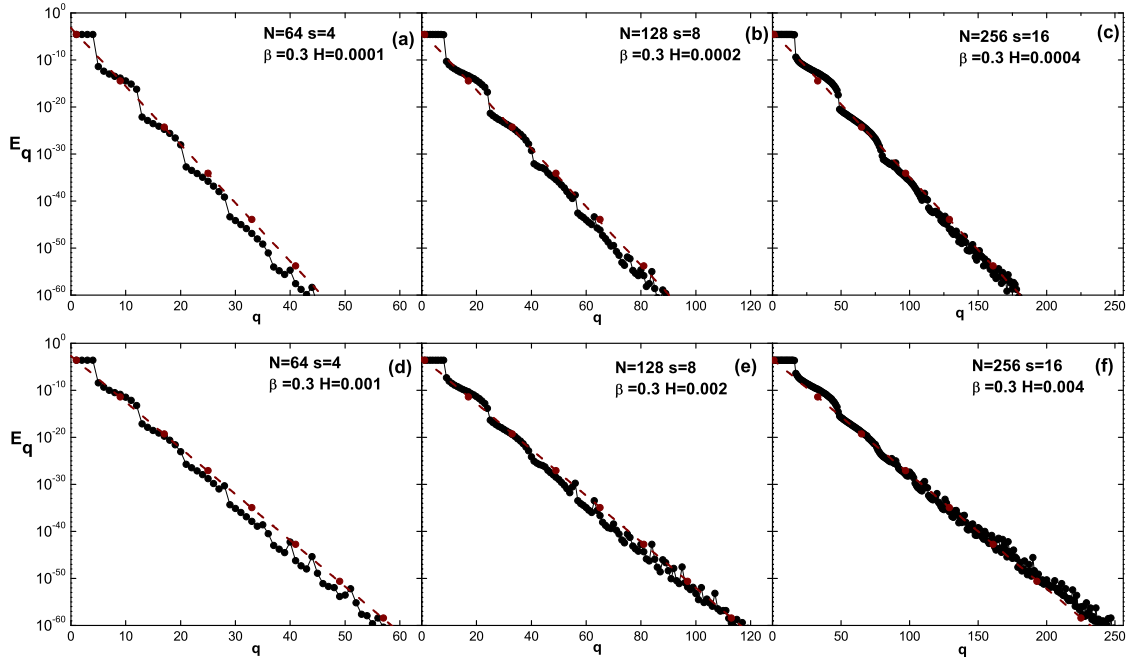


Fig. 9. The average harmonic energy E_q of the q -th mode over a time span $T = 10^6$ as a function of q in various examples of FPU-trajectories, for $\beta = 0.3$, in which the $s(= N/16)$ first modes are only excited initially via $Q_q(0) = A_q$, $\dot{Q}_q(0) = 0$, $q = 1, \dots, s$, with the A_q selected so that the total energy is equal to the value $E = H$ indicated in each panel. We thus have (a) $N = 64$, $E = 10^{-4}$, (b) $N = 128$, $E = 2 \times 10^{-4}$, (c) $N = 256$, $E = 4 \times 10^{-4}$, (d) $N = 64$, $E = 10^{-3}$, (e) $N = 128$, $E = 2 \times 10^{-3}$, (f) $N = 256$, $E = 4 \times 10^{-3}$. The specific energy is constant in each of the two rows, i.e. $\varepsilon = 1.5625 \times 10^{-6}$ in the top row and $\varepsilon = 1.5625 \times 10^{-5}$ in the bottom row. The dashed lines represent the average exponential profile E_q obtained theoretically by the hypothesis that the depicted FPU trajectories lie close to q -tori governed by the profile (120).

(for $N = 256$) first modes are excited at $t = 0$, with the excitation amplitudes being compatible with the values of the total energy E indicated in each panel, specific energy $\varepsilon = 1.5625 \times 10^{-6}$ in the top row and $\varepsilon = 1.5625 \times 10^{-5}$ in the bottom row of Fig. 9. Thus, these FPU trajectories can be considered as lying in the neighborhood of the q -torus solutions, at least initially. The numerical evidence is that if E is small, they remain close to the q -tori even after relatively long times, e.g. $t = 10^6$.

This is evident in Fig. 9, in which one sees that the average energy profiles of the FPU-trajectories (at $t = 10^6$) exhibit the same behavior as predicted by Eq.(118), for an exact q -torus solution with the same total energy as the FPU trajectory in each panel. For example, based on the values of their average harmonic energy, the modes in Fig. 9a (in which $s = 4$) are clearly separated in groups, (1 to 4), (5 to 12) and (13 to 20), etc., as predicted theoretically for an exact 4-torus solution. The energies of the modes in each group have a sigmoid variation around a level value characteristic of the group, which is nearly the value predicted by Eq.(118). Also, if we superpose the numerical data of the three top (or bottom) panels we find that the average exponential slope is nearly identical in all panels of each row, as implied by Eq.(120), according to which, for a given fraction M of initially excited modes, this slope depends on the specific energy only, and is independent of N .

Of course, when the energy is increased, the FPU-trajectories resulting from s initially excited modes start to deviate from their associated tori, when these become *unstable*. As a consequence, the energy profiles of the FPU-trajectories also start to deviate from the energy profiles of the exact s -tori. This is shown in Fig. 10a by the fact that the profiles of the FPU-trajectories become smoother and the groups of modes less distinct, when the energy increases by a factor 50 (with respect to Fig. 9d), for the same values of N and β . We also observe in Fig. 10a–f the formation of the so-called ‘tail’, i.e. an overall rise of the localization profile at the high-frequency part of the spectrum. This is a precursor of the evolution of the system towards equipartition, which ultimately sets in at high enough energy.

This exponential localization of energy profiles also occurs in FPU particle chains, when p.b.c. are

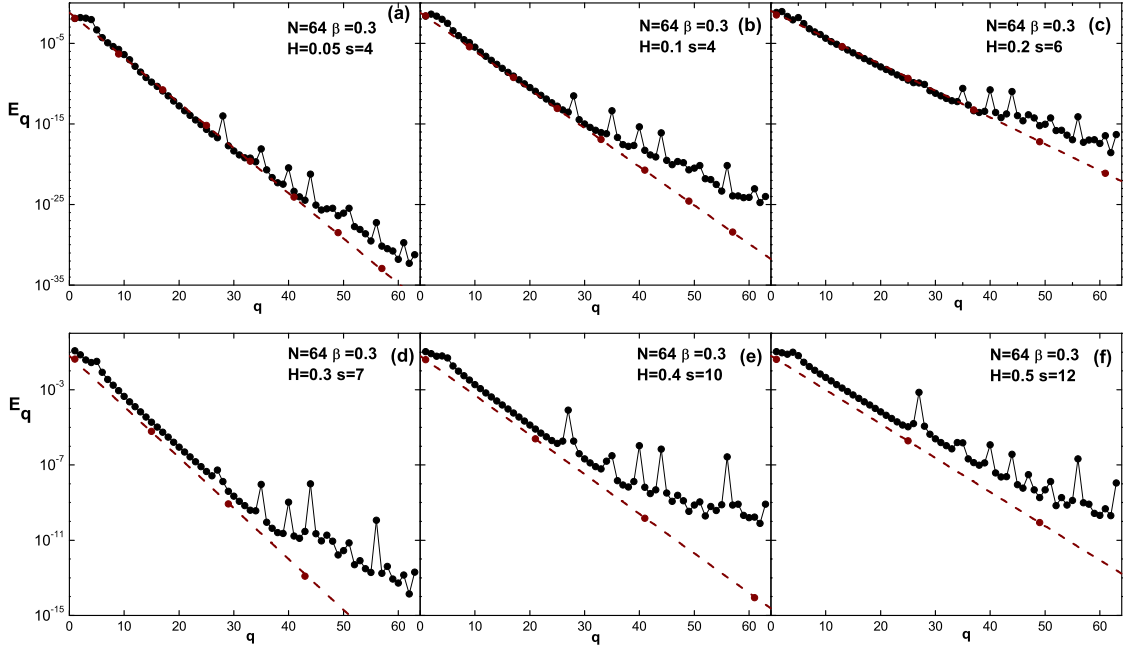


Fig. 10. Same as in Fig.9a but for larger energies, namely (a) $E = 0.05$, (b) $E = 0.1$, (c) $E = 0.2$, (d) $E = 0.3$, (e) $E = 0.4$, (f) $E = 0.5$. Beyond the threshold $E \simeq 0.05$, theoretical profiles of the form (118) yield the correct exponential slope if s is gradually increased from $s = 4$ in (a) and (b) to $s = 6$ in (c), $s = 7$ in (d), $s = 10$ in (e), and $s = 12$ in (f).

imposed. In fact, the profiles in this case become perfectly symmetric with respect to the middle modes if one respects the symmetry of the (linear) normal mode spectrum, (107), and excites equally the q mode *and* $N - q$ mode, which have the same frequency, see Fig. 11. The existence and stability of the corresponding q -tori at low energies is also evident here and is expected to play an equally important role in the phenomenon of FPU recurrences, as in the case of the fixed boundary conditions.

4.2. Stability of the motion on q -tori and the GALI method

As we have frequently emphasized, one of the most important properties concerning the dynamics of conservative mechanical systems, is whether the motion is “regular” or “predictable” for a given set of parameters and initial conditions. Since stable periodic orbits are a set of measure zero, this typically implies that the solutions we seek are quasiperiodic in time. In N -degree-of-freedom Hamiltonian models, quasiperiodic orbits are generically located around stable periodic orbits and lie on N -dimensional tori.

In particular, when studying the phenomenon of FPU recurrences in subsection IV.A, we realized that it is crucial to follow NNMs with low wave numbers $q = 1, 2, 3, \dots$. These are simple periodic solutions called q -breathers (due to their exponential localization in q -space), whose initial conditions are very close to those of the recurrent FPU trajectories. Owing to this proximity, one might expect that as long as q -breathers are stable recurrences will continue for arbitrarily long times.

In fact, the situation is somewhat more complicated. The reason is that exponential localization in q -space is also a property shared by the tori surrounding these NNMs, which we called q -tori in subsection IV.A. Actually it is *their* stability that matters and not that of the q -breathers, since, as the energy increases, q -tori are seen to persist even after the NNMs at their midst have turned unstable!

Of course, the stability of q -breathers can be studied by Floquet theory, as shown e.g. in [Flach *et al.*, 2006], where it was demonstrated that q -breathers with low $q = q_0 = 1, 2, 3, \dots$ are linearly stable as long as

$$E_{q_0} \leq \frac{\pi^2}{6\beta(N+1)} + O(1/N^2) \quad (121)$$

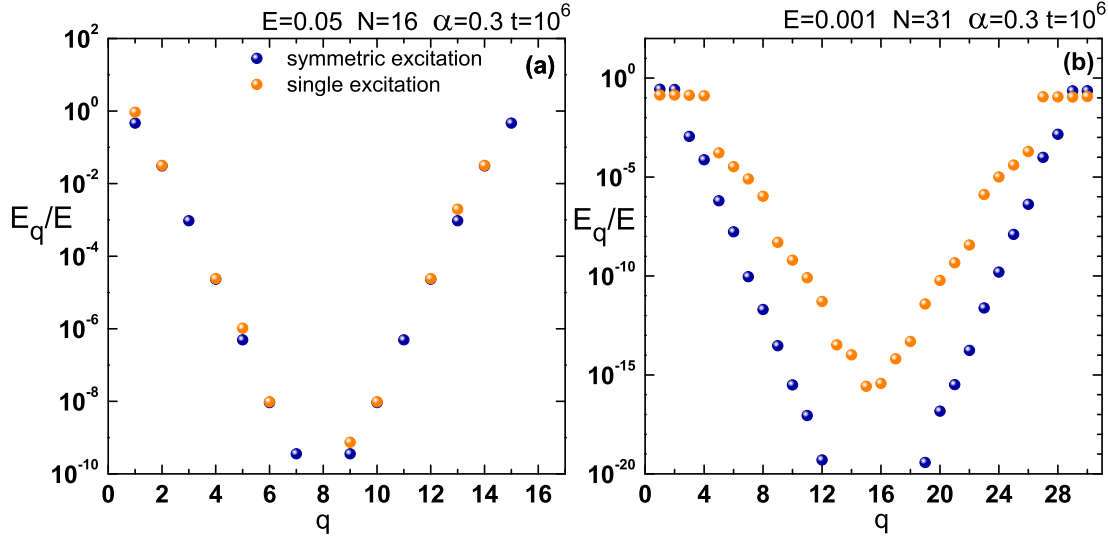


Fig. 11. The average harmonic energy E_q of the q -th mode as a function of q for the FPU- α model with $\alpha = 0.3$ and $\beta = 0$ in (99) evaluated after a time $T = 10^6$. (a) A q -breather with $N = 16$ is shown at energy $E = .05$ is (b) and a 2-torus and 4-torus solution with $N = 31$ are depicted at energy $E = .001$. Note that in (a), when only the $q = 1$ mode is excited, the profile is not as symmetric as it becomes when *both* $q = 1$ and $q = N - 1$ modes are excited equally.

This result is obtained by analyzing the eigenvalues of the monodromy matrix of the linearized equations about a q -breather constructed by the Poincaré - Lindstedt series. Furthermore, examining also the associated eigenvectors one gains a complete understanding of the tangent dynamics in the vicinity of these simple periodic orbits.

In the case of q -tori, however, the above techniques are no longer available. Stability is not decided by the eigenvalues of a solution matrix and one must seek different ways of exploring the variational equations linearized about quasiperiodic orbits. One analytical approach for example, described in section III, is to use discrete symmetries of the system to write the linearized equations in the simplest form, expanding the solutions in terms of linear combinations of NNMs, so that they “uncouple” as much as possible.

Interesting as this approach may be, a more accurate stability analysis should focus on the full set of variational equations and examine the behavior of their solutions for *arbitrary* choices of initial conditions. This can be achieved by employing the recently proposed method of the Generalized Alignment Indices (GALI), which we outline below (see [Skokos *et al.*, 2008]):

Consider an orbit $\gamma(t) = (\mathbf{p}(t), \mathbf{q}(t))$, representing a solution of the Hamiltonian equations of motion (1) with initial conditions $(\mathbf{p}(0), \mathbf{q}(0))$. The variational equations along this orbit describe the dynamics on the tangent space of the solutions of (1) and are given by the vector field

$$\frac{d\mathbf{w}}{dt} = J \cdot M(\mathbf{p}(t), \mathbf{q}(t))\mathbf{w} \quad (122)$$

where $J = \begin{pmatrix} O & I_N \\ -I_N & O \end{pmatrix}$, I_N the $N \times N$ unit matrix and $M(\mathbf{p}(t), \mathbf{q}(t))$ is the Hessian matrix of the Hamiltonian function evaluated along $\gamma(t)$, i.e.

$$M(\gamma(t)) = \frac{\partial^2 H}{\partial \mathbf{p} \partial \mathbf{q}} \Big|_{\gamma(t)} \quad (123)$$

Let us now solve equations (122) for $\mathbf{w}_1(t)$, $\mathbf{w}_2(t)$, ..., $\mathbf{w}_k(t)$, using as initial conditions k randomly chosen orthocanonical vectors and construct the unit vectors

$$\hat{w}_i = \frac{\mathbf{w}_i}{\|\mathbf{w}_i\|}, \quad i = 1, \dots, k \quad (124)$$

The Generalized Alignment Index $GALI_k(t)$ is defined at time t as the *volume* of the parallelepiped produced by these k unit deviation vectors \hat{w}_i , $i = 1, \dots, k$ expressed, at time t , by the wedge product

$$GALI_k(t) = \|\hat{w}_1 \wedge \hat{w}_2 \wedge \dots \wedge \hat{w}_k\| \quad (125)$$

As is well-known, this wedge product can be written with respect to the basis \hat{e}_{i_k} in the form

$$\hat{w}_1 \wedge \hat{w}_2 \wedge \dots \wedge \hat{w}_k = \sum_{1 \leq i_1 < i_2 < \dots < i_k \leq 2N} \begin{vmatrix} w_{1i_1} & w_{1i_2} & \dots & w_{1i_k} \\ w_{2i_1} & w_{2i_2} & \dots & w_{2i_k} \\ \vdots & \vdots & & \vdots \\ w_{ki_1} & w_{ki_2} & \dots & w_{ki_k} \end{vmatrix} \hat{e}_{i_1} \wedge \hat{e}_{i_2} \wedge \dots \wedge \hat{e}_{i_k} \quad (126)$$

From this it is easy to see that if at least two of the normalized deviation vectors \hat{w}_i , $i = 1, 2, \dots, k$ are linearly dependent, all the $k \times k$ determinants will become zero and the volume will vanish. Clearly, the norm of this quantity, $\|\hat{w}_1(t) \wedge \hat{w}_2(t) \wedge \dots \wedge \hat{w}_k(t)\|$, is obtained by evaluating the sums

$$GALI_k(t) = \left\{ \sum_{1 \leq i_1 < i_2 < \dots < i_k \leq 2N} \left| \begin{vmatrix} w_{1i_1} & w_{1i_2} & \dots & w_{1i_k} \\ w_{2i_1} & w_{2i_2} & \dots & w_{2i_k} \\ \vdots & \vdots & & \vdots \\ w_{ki_1} & w_{ki_2} & \dots & w_{ki_k} \end{vmatrix} \right|^2 \right\}^{1/2} \quad (127)$$

As was described in detail in a number of papers [Skokos *et al.*, 2007, 2008; Christodoulidi & Bountis, 2006], it is possible to analyze the *asymptotic* behavior of these sums by estimating the largest determinants as $t \rightarrow \infty$, both for chaotic as well as quasiperiodic motion. Thus, the following asymptotic estimates are derived:

I) For chaotic orbits:

$$GALI_k(t) \propto e^{-[(\sigma_1 - \sigma_2) + (\sigma_1 - \sigma_3) + \dots + (\sigma_1 - \sigma_k)]t}. \quad (128)$$

where

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_{N-1} \geq \sigma_N = \sigma_{N+1} = 0 \geq \sigma_{N+2} \geq \dots \geq \sigma_{2N}. \quad (129)$$

are the Lyapunov exponents of the orbit [Skokos, 2010].

II) For quasiperiodic orbits lying on an s -dimensional torus:

$$GALI_k(t) \sim \begin{cases} \text{constant} & \text{if } 2 \leq k \leq s \\ \frac{1}{t^{k-s}} & \text{if } s < k \leq 2N - s \\ \frac{1}{t^{2(k-N)}} & \text{if } 2N - s < k \leq 2N \end{cases}. \quad (130)$$

In the “generic case” $s = N$, (130) implies that the $GALI_k$ remain constant for $2 \leq k \leq N$ and decrease to zero as $\sim 1/t^{2(k-N)}$ for $N < k \leq 2N$. However, as we have seen in this review, the “non-generic” case of low-dimensional tori, with $s \ll N$, is also of great physical interest and occurs quite frequently in mechanical systems of the type considered here.

The accuracy of the above formulas, when compared against numerical experiments, is remarkable. Indeed, as has been demonstrated in many papers [Skokos *et al.*, 2007, 2008; Bountis *et al.*, 2008; Christodoulidi & Bountis, 2006] the $GALI_k$ reach their asymptotic values after relatively short times. In the chaotic case, the indices follow very closely the theoretical values even when the Lyapunov exponents (and their differences) are very small and have not as yet converged to their limiting values. Indeed, it is important to note that what makes the GALI method so efficient in distinguishing chaos from order is the fundamental difference between exponential and power law decay. In the case of chaotic orbits, *all* indices decrease exponentially and chaos is most quickly detected by inspecting the ones with high k values, while for quasiperiodic orbits all $GALI_k$ decrease by power laws, except for the first few which are nearly constant and signify the dimension of the torus.

Concerning the calculation of the $GALI_k$, it is clear that, for large N , the computations become prohibitively time-consuming, due to the number and size of determinants in (127). There is, however, a

much faster way to proceed: Observe that the normalized deviation vectors \hat{w}_i , $i = 1, 2, \dots, 2N$, discussed above, when expressed in terms of the usual orthonormal basis of the n -dimensional Euclidian space can be written as

$$\hat{w}_i = \sum_{j=1}^{2N} w_{ij} \hat{e}_j, \quad i = 1, 2, \dots, k \quad (131)$$

Thus, we can write equations (131) in matrix form as:

$$\begin{bmatrix} \hat{w}_1 \\ \hat{w}_2 \\ \vdots \\ \hat{w}_k \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1,2N} \\ w_{21} & w_{22} & \cdots & w_{2,2N} \\ \vdots & \vdots & & \vdots \\ w_{k1} & w_{k2} & \cdots & w_{k,2N} \end{bmatrix} \cdot \begin{bmatrix} \hat{e}_1 \\ \hat{e}_2 \\ \vdots \\ \hat{e}_{2N} \end{bmatrix} = \mathbf{A} \cdot \begin{bmatrix} \hat{e}_1 \\ \hat{e}_2 \\ \vdots \\ \hat{e}_{2N} \end{bmatrix}. \quad (132)$$

Recall that GALI_k measures the volume of a k -parallelepiped P_k having as edges the k unitary deviation vectors \hat{w}_i , $i = 1, \dots, k$. This volume is given by ([Hubbard & Hubbard, 1999]):

$$\text{vol}(P_k) = \sqrt{\det(\mathbf{A} \cdot \mathbf{A}^T)}, \quad (133)$$

since $\det(\mathbf{A} \cdot \mathbf{A}^T)$ is equal to the sum appearing in (127) by virtue of Lagrange's identity [Bourbaki, 1958] (where $(^T)$ denotes transpose). Thus we obtain a much more efficient way of computing GALI_k by the formula:

$$\text{GALI}_k = \sqrt{\det(\mathbf{A} \cdot \mathbf{A}^T)}, \quad (134)$$

where only the multiplication of two matrices and the square root of one determinant appears.

Let us see how one can apply the above spectrum of indices to the problems considered in this review. First of all, we have already seen the usefulness of the GALI_k in determining the dimensionality of the q -tori described in subsection IV.A, see Fig. 7d and the discussion below it. Indeed, the near constancy of the GALI_k , for $k = 1, 2, \dots, s$, at least for the time intervals studied, is always seen to characterize stable tori formed by exciting s linear normal modes of our FPU chains, at low energies.

Quasiperiodic tori, however, can become *unstable* by losing their smoothness and eventually breaking down into sets of points called cantori [MacKay & Meiss, 1987]. This means that the variational equations about them possess a non-empty unstable manifold through which small variations about the torus are expected to grow exponentially. It follows, therefore, that beyond the critical energy at which a q -torus becomes unstable, all deviation vectors lying on the unstable manifold will tend to align in the direction with the largest exponent, making all GALI indices fall exponentially fast. Thus, the instability of the torus can be verified, e.g. following the $k = 2$ index, GALI_2 , which is the fastest to compute, even though the indices for higher k values tend more quickly to zero.

Using this criterion, it is easy to test the stability of q -tori and determine approximately the value of the critical energy E_c at which they become unstable. Fig. 12 shows an example of such a calculation using trajectories started close to a 3-torus (upper curve), 2-torus (middle curve), together with one starting close to a q -breather (lower curve) for fixed β . Observing the dependence of this instability threshold on N , we discover that the E_c values of at which the q -tori destabilize are significantly *higher* than those corresponding to the destabilization of q -breathers.

This is also inferred from the fact that the square and triangle data in Fig. 12 show a much weaker dependence of A on N than the N^{-1} law predicted by (121) for q -breathers. The relation $A \propto N^{-1}$ is seen to hold well only for FPU-trajectories started close to a q -breather with $q = 1$ (filled circles), whose numerical curve is close to the dashed line predicted by Eq.(121). These results strongly suggest that the critical thresholds E_c at which q -tori (obtained by exciting the low modes) break down are significantly higher than the energies at which the corresponding q -breathers become unstable.

We, therefore, conclude this section by emphasizing that perhaps the most important feature concerning the dynamics of orbits forming q -breathers or q -tori is the exponential localization of their energies, which persists even after these solutions have become linearly unstable. This behavior is exemplified in Figure

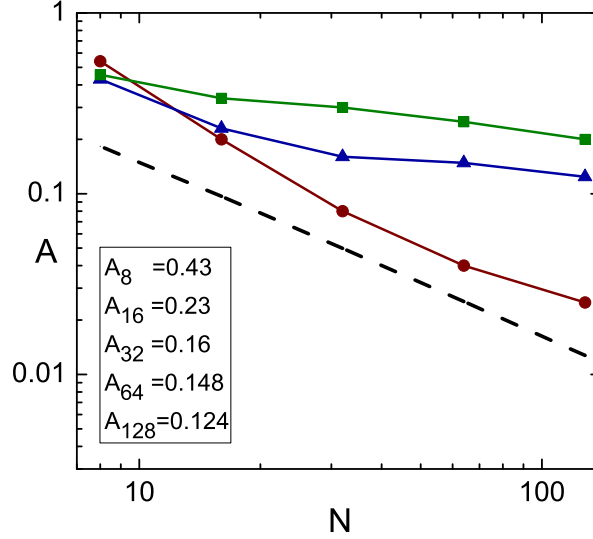


Fig. 12. Fixing β we plot in the upper curve (squares) the dependence of the mean oscillation amplitude A on N , for critical energies E_c determined by the destabilization of a 3-dimensional q -torus for FPU-trajectories identified as quasiperiodic by teh $\text{GALI}_k = \text{const.}$ for $k = 1, 2, 3$. The middle curve (triangles) corresponds to a similar calculation for an FPU trajectory started by exciting initially a 2-dimensional q -torus, while the lower one (circles) refers to a q-breather solution ($q_0 = 1$). The dashed line represents the law of Eq.(121) and all calculations are carried out up to $t = t_{\max} = 10^7$.

13, where panels (a) and (c) show the time evolution of the GALI_2 index for two FPU trajectories started in the vicinity of 2-tori of FPU- β systems with $N = 32$ and $N = 128$, for $\beta = 0.1$ and $t_{\max} = 10^7$. In both cases, the energy satisfies $E > E_c$, as the exponential decay of the GALI_2 index evidently shows and the corresponding q -tori are unstable. Still, as Figs. 13b,d clearly demonstrate, the exponential localization of the energies, at least for the lower part of the spectrum, holds in this case also.

This localization property of the q -tori, therefore, provides, in our view, a more complete interpretation of the phenomenon of FPU recurrences. If there is still something “paradoxical” about it, it is that it is not known to date if it holds to $t \rightarrow \infty$, for small but non-zero energies. What is certainly true (as Figs. 13b,d show) is that the destabilization of the q -tori brings about the *delocalization* of *higher* q -modes and the break down of recurrences, signifying the eventual equipartition of energy, which is expected to spread to all modes at $t > T_{eq}(\epsilon)$, where $\epsilon = E/N$ is the specific energy and become practically observable when ϵ is large enough.

Appendix A

5. Elements of group representation theory

5.1. Natural representation

We begin with an especially useful representation, called here *natural representation* of the parent group, using as an example the square molecule model, depicted in Fig. 2. We can describe the atomic displacement patterns of the vibrational states of this molecule at any fixed time t by eight-dimensional configuration vectors of the form

$$\vec{X} = \{\vec{r}_1 | \vec{r}_2 | \vec{r}_3 | \vec{r}_4\} = \{x_1, x_2 | x_3, x_4 | x_5, x_6 | x_7, x_8\}. \quad (\text{A.1})$$

where x_1, x_2 are displacements of the first atom from the equilibrium position (see Fig. 2) along the axes X and Y , while $\{x_3, x_4\}$, $\{x_5, x_6\}$, $\{x_7, x_8\}$ are those of the atoms 2, 3 and 4, respectively.

Let us act on an instantaneous vibrational configuration of the molecule by a certain symmetry element g_i , see Eqs.(41). Actually, we must act on the *displaced* atoms whose coordinates are determined by vectors

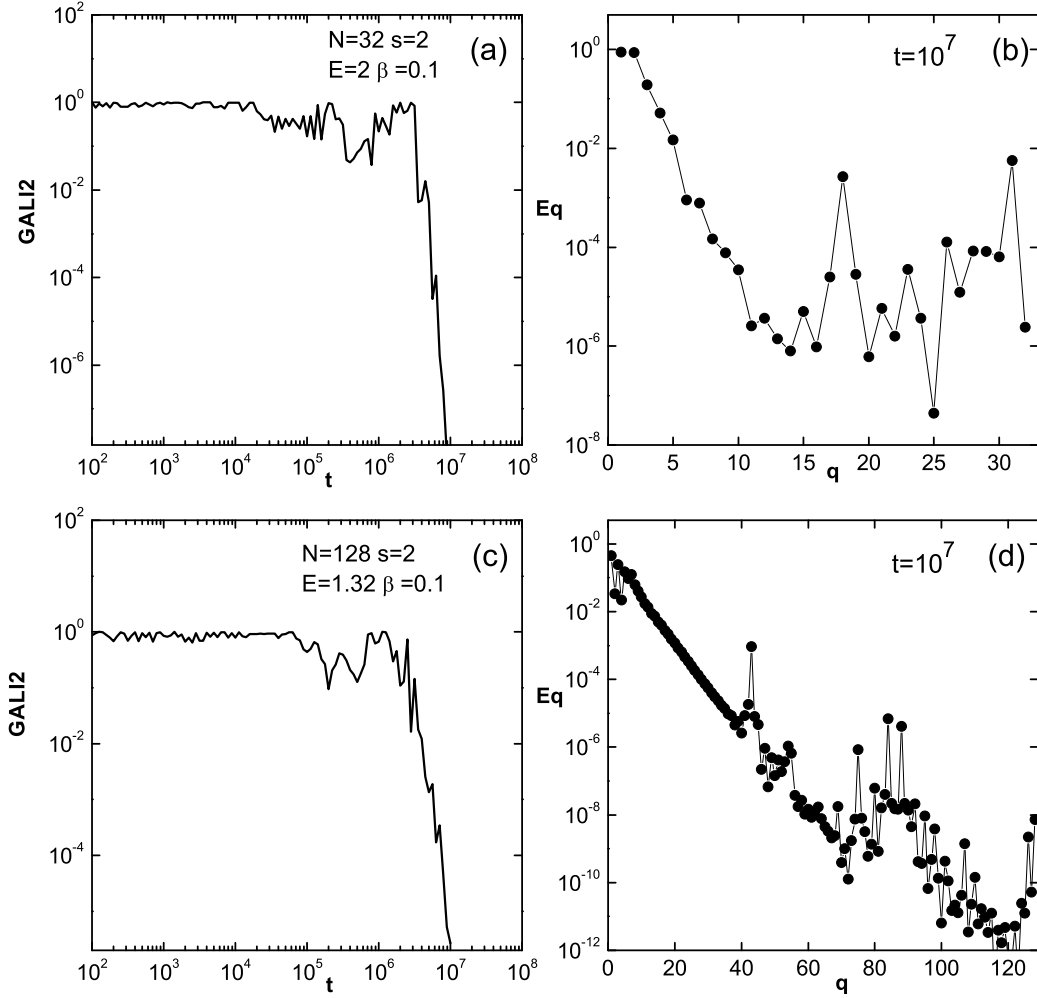


Fig. 13. (a) Time evolution of the GALI_2 index up to $t = 10^7$ for an FPU trajectory started by exciting the $q = 1$ and $q = 2$ modes in the system $N = 32$, $\beta = 0.1$, with total energy $E = 2$, i.e. higher than $E_c = 1.6$. (b) *Instantaneous* localization profile of the FPU trajectory of (a) at $t = 10^7$. (c) Same as in (a) but for $N = 64$, $E = 1.323$ (in this case the critical energy is $E_c = 1.24$). (d) Same as in (b) but for the trajectory of (c).

$\vec{R}_j = \vec{R}_j^0 + \vec{r}_j$, where $\vec{R}_j^0 = (x_j^0, y_j^0)$ is the equilibrium position of the j -th atom, while $\vec{r}_j = (x_j, y_j)$ is the local vector which determines the displacement of this atom from its equilibrium position.

Since $g_i \vec{R}_j = g_i \vec{R}_j^0 + g_i \vec{r}_j$, one can introduce *operators* \hat{g}_i , which are *induced* by the symmetry elements $g_i \in G_0$, acting on the eight dimensional configuration vector (A.1) by the following two step process:

- 1) *transpose* the local displacement vectors $\vec{r}_j = (x_j, y_j)$ in (A.1) according to the transposition of atom equilibrium positions under the action of the symmetry element g_i^{-1} ;
- 2) *act* on each local displacement vector \vec{r}_j by the symmetry element g_i^{-1} .

For example, we obtain for the symmetry element g_2 :

$$\hat{g}_2 \vec{X} = \{g_4 \vec{r}_2 | g_4 \vec{r}_3 | g_4 \vec{r}_4 | g_4 \vec{r}_1\} = \{y_2, -x_2 | y_3, -x_3 | y_4, -x_4 | y_1, -x_1\}, \quad (\text{A.2})$$

⁴Note that symmetry element g acts on the vectors \vec{r} of three-dimensional Euclidean space, while operator \hat{g} acts on vectors of the eight-dimensional configuration space. In general, the induced operator \hat{g} , acting on an arbitrary function $f(\vec{r})$, is determined by the equation $\hat{g}f(\vec{r}) = f(g^{-1}\vec{r})$, as shown in any textbook on the theory of symmetry groups (see, for example, [Hammermesh, 1962; Elliott & Dawber, 1979]).

taking into account relations $g_2^{-1} = g_4$ and $g_4(x, y) = (y, -x)$ (g_2 and g_4 are rotations about the Z axis through the angles 90° and 270° , respectively).

The above definition of the operators \hat{g}_i induced by symmetry elements g_i allows one to construct an eight-dimensional natural representation of the symmetry group $G_0 = C_{4v}$ for the considered square molecule. To this end, we may choose the “natural” basis $\vec{\Phi} = \{\vec{e}_1, \vec{e}_2, \dots, \vec{e}_N\}$ of orthogonal unit vectors \vec{e}_i (having 1 in their i th entry and zero everywhere else) to describe all possible displacements in the configuration space.

Next, acting by an operator \hat{g} ($g \in G_0$) on the vector \vec{e}_j , we can write $\hat{g}\vec{e}_j$ as a certain linear combination of all basis vectors:

$$\hat{g}\vec{e}_j = \sum_{i=1}^N \mathcal{M}_{ij}(g)\vec{e}_i, \quad j = 1, 2, \dots, N. \quad (\text{A.3})$$

This equation associates the matrix $\mathcal{M}(g) = \{\mathcal{M}_{ij}(g)\}$ with the operator \hat{g} and, therefore, with the symmetry element $g \in G_0$:

$$g \Rightarrow \hat{g} \Rightarrow \mathcal{M}(g). \quad (\text{A.4})$$

The set of matrices $\mathcal{M}(g)$ corresponding to all $g \in G_0$ forms the natural representation Γ for our mechanical system.

In the case of the square molecule, $N = 8$, therefore, this representation turns out to be eight-dimensional — and represents a collection of 8×8 matrices $\mathcal{M}(g)$ which correspond to all the elements g of the parent group G_0 .

Moreover, these matrices satisfy the same multiplication rule as the symmetry elements corresponding to them: if $g_i g_j = g_k$, then $M(g_i) \cdot M(g_j) = M(g_k)$. Among them there is the unit matrix [$M(g_1) = I$], and for every matrix there also exists its inverse [$M(g^{-1}) = M^{-1}(g)$]. Taking into account the associative rule for matrix multiplication, we can show that all different matrices belonging to the set $\{M(g) | \forall g \in G_0\}$ generate a certain *matrix group homeomorphic* to the parent group G_0 (In general, a matrix representation can contain a number of identical matrices).

It is well-known that any finite group possesses an infinite number of representations whose dimensions can be arbitrarily large. However, there exists only a *finite number* of nonequivalent *irreducible representations* (irreps). Let us consider this issue in more detail.

5.2. Irreducible representations

Let us first use the basis $\Phi = \{\vec{e}_1, \dots, \vec{e}_N\}$ to construct the natural representation of the parent group $G_0 = C_{4v}$. Of course, one may use any other basis of the configuration space for the same purpose. This leads to considering a new form of matrices corresponding to symmetry elements $g \in G_0$ as follows:

$$M_{\text{new}}(g) = S^{-1}M(g)S, \quad \forall g \in G_0. \quad (\text{A.5})$$

where S is a non-singular matrix. Based on this idea, we may ask: “How can one choose the basis of our configuration space to make the matrices $M(g)$ of the natural representation as simple as possible?”

Indeed, let us recall that if a number of matrices commute with each other they can be transformed to the simplest possible — *diagonal* — form via a transformation of the type (A.5), using a suitably chosen matrix S . On the other hand, if the matrices do not commute, they cannot be diagonalized simultaneously by transformation of the form (A.5), i.e. such a matrix S does not exist.

The natural representation is only one example of a matrix representation of a given symmetry group. Continuing our discussion of arbitrary matrix representations of finite groups, we now consider representations Γ_j of the group G by complex $n \times n$ matrices $\mathcal{M}(g), g \in G$. These matrices act on the vectors of an n -dimensional complex vector space which is called the *carrier* space of Γ .

In physics, we usually deal with *unitary* representations [Hammermesh, 1962; Elliott & Dawber, 1979]. All matrices $\mathcal{M}(g)$ of such representations are unitary matrices, satisfying $\mathcal{M}^\dagger(g) = \mathcal{M}^{-1}(g), \forall g \in G$.

Definition A.1. Two matrix representations $\Gamma = \{ \mathcal{M}(g) \mid g \in G \}$ and $\Gamma' = \{ \mathcal{M}'(g) \mid g \in G \}$ of the group G are called *unitary equivalent*, if there exists a unitary matrix S (i.e. $S^\dagger = S^{-1}$), such that all their matrices obey the relation

$$\mathcal{M}'(g) = S^\dagger \mathcal{M}(g) S, \quad (\text{A.6})$$

The transformation (A.6) appears when we pass from one orthonormal basis of the carrier space of a given representation to another. Let us now define the matrix representation Γ associated with a certain basis $\vec{\Phi} = \{ \vec{\varphi}_1(\vec{r}), \vec{\varphi}_2(\vec{r}), \dots, \vec{\varphi}_n(\vec{r}) \}$ of the carrier space:

Definition A.2. If

$$\hat{g}\vec{\Phi} = \widetilde{\mathcal{M}}(g)\vec{\Phi} \quad (\text{for all } g \in G), \quad (\text{A.7})$$

where operator \hat{g} acts on the basis vectors $\vec{\varphi}_j(\vec{r})$ as $\hat{g}\vec{\varphi}_j(\vec{r}) = \vec{\varphi}_j(g^{-1}\vec{r})$, then

$$\Gamma = \{ \mathcal{M}(g) \mid \forall g \in G \} \quad (\text{A.8})$$

is a matrix representation of the group G . Note that $\widetilde{\mathcal{M}}(g)$ denotes the transpose of the matrix $\mathcal{M}(g)$.

Let us also denote by the symbol V the carrier space of the matrix representation Γ of the group G and suppose we can write V as a *direct sum*

$$V = \sum_{j=1}^K V_j \quad (\text{A.9})$$

of a number $K > 1$ of *invariant subspaces* V_j , which are *independent* of each other under the action of operators \hat{g} induced by all the elements of the group G . More precisely the above invariance can be explained as follows: Each operator \hat{g} ($g \in G$) acting on any vector \vec{v} belonging to V_j transforms it into another vector of the *same subspace*, i.e. $\hat{g}\vec{v}$ cannot *coincide* with a vector of any other subspace in the sum (A.9) different from V_j .

If we choose an arbitrary basis in the subspace V_j , we obtain a matrix representation Γ_j of the group G which is constructed on this basis according to the general definition (A.7,A.8).

Since the basis of the full space V can be chosen as the union of all subspaces V_j entering Eq. (A.9), we find that the representation Γ can be written as a *direct sum* of all the representations Γ_j constructed using the bases of the individual subspaces V_j :

$$\Gamma = \sum_{j=1}^N \oplus \Gamma_j. \quad (\text{A.10})$$

The dimension n of the full carrier space V is the sum of the dimensions n_j of all its invariant subspaces V_j :

$$n = \sum_{j=1}^N n_j. \quad (\text{A.11})$$

If a subspace V_j *cannot* be split into invariant subspaces of *smaller* dimensions, it is called *irreducible* and so is the representation Γ_j , defined on it. On the other hand, the representation Γ , defined on the full space V is called "reducible", if it can be decomposed into a finite number of $K > 1$ irreducible representations.

As a consequence of Eq. (A.10), a reducible representation Γ possesses *block diagonal* form, whose blocks turn out to be the individual irreducible representation Γ_j . For the given matrix $D_i(g) \in \Gamma_i$, each of these blocks, $\mathcal{D}_{nj}^{(i)}(g)$, represents an $n \times n$ matrix corresponding to $g \in G$, while i numbers the blocks of one and the same dimension (n). Observe that, when a certain irrep Γ_j is contained in the reducible representation Γ a number of times m_j (the subduction frequency), some blocks may be identical.

We may, therefore, rewrite equation (A.10) in the form:

$$\Gamma = \sum_j^{\oplus} m_j \Gamma_j, \quad (\text{A.12})$$

where m_j indicates how many times the irrep Γ_j is contained in the decomposition of the reducible representation Γ . Let us note that the basis vectors of different copies of the same irrep Γ_j are essentially *different*. One should also emphasize that matrices of all irreps Γ_j must be known to obtain the explicit decomposition of the given reducible representation, while for the *schemes of the decomposition* (A.12) one needs to know only the *characters* of these irreps.

Definition A.3. A character $\bar{\chi}[\Gamma]$ of the n -dimensional representation is the n -dimensional vector constructed by the *traces* of all the matrices $\mathcal{M}(g)$ of this representation:

$$\bar{\chi}[\Gamma] = \frac{1}{\sqrt{\|G\|}} \{ \text{Tr} \mathcal{M}(g) \mid g \in G \},$$

where $\|G\|$ denotes the order of the group G .

There exists a powerful group theoretical apparatus using the irreps and their characters for solving a wide class of crystal and molecular systems. The characters of the irreps of a given group are orthonormal vectors. For calculating the subduction frequency m_j of the irrep Γ_j from Eq. (A.12), one can use the following formula [Hammermesh, 1962; Elliott & Dawber, 1979]:

$$m_j = (\bar{\chi}[\Gamma], \bar{\chi}[\Gamma_j]) \equiv \frac{1}{\|G\|} \sum_{g \in G} \chi_{\Gamma}(g) \bar{\chi}_j(g). \quad (\text{A.13})$$

Here $\bar{\chi}[\Gamma]$ is the character of the reducible representation Γ , while $\bar{\chi}[\Gamma_j]$ is the character of the irreducible representation Γ_j ($\bar{\chi}[\Gamma_j]$ is the complex conjugate value with respect to $\bar{\chi}[\Gamma_j]$).

5.3. Some properties of irreducible representations and their role in Physics

Irreducible representations (irreps) possess many remarkable properties which can be found in any textbook on group theory (see, for example, [Hammermesh, 1962; Elliott & Dawber, 1979]). In particular, it is well-known that any group G of finite order $\|G\|$ possesses a *finite number* of different nonequivalent irreps, and this number is equal to the number of classes of conjugate elements of the given group. The dimension (n_j) of each irrep (Γ_j) must be a divisor of the group order $\|G\|$, i.e. $\|G\| \bmod n_j = 0$. Dimensions of all the irreps of the group G satisfy the Burnside theorem:

$$\sum_{j=1}^N n_j^2 = \|G\|. \quad (\text{A.14})$$

Among irreps of any group G there is the so-called *identity* representation which associates with every element $g \in G$ one and the same one-by-one unit matrix.

Let us now return to the group $G = C_{4v}$ of the square molecule. The order $\|G\|$ of this group is equal to 8 (all its elements are listed in Eq.(41)). According to Eq. (A.14) there exist only three variants for the possible set of dimensions of the irreps of the group $G = C_{4v}$:

$$2^2 + 2^2 = 8, \quad (\text{A.15})$$

$$1^2 + 1^2 + 1^2 + 1^2 + 1^2 + 1^2 + 1^2 + 1^2 = 8, \quad (\text{A.16})$$

$$1^2 + 1^2 + 1^2 + 1^2 + 2^2 = 8. \quad (\text{A.17})$$

In variant (A.15), there are two 2-dimensional irreps ($n_1 = 2, n_2 = 2$). This is impossible because any group must possess *at least* one 1-dimensional irrep : the identity irrep. Variant (A.16) ($n_j = 1, j = 1 \dots 8$) is also impossible because only for Abelian group *all* the irreps can be 1-dimensional, while the group $G = C_{4v}$ is non-Abelian. Therefore, only variant (A.17) turns out to be admissible: the group $G = C_{4v}$

possesses *five* irreps : four 1-dimensional ($n_1 = n_2 = n_3 = n_4 = 1$) and one 2-dimensional ($n_5 = 2$), as presented in Table 1 below.

Table 1. Symmetry elements of the group G and their irreps

	g_1	g_2	g_3	g_4	g_5	g_6	g_7	g_8
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	-1	-1	-1	-1
Γ_3	1	-1	1	-1	1	-1	1	-1
Γ_4	1	-1	1	-1	-1	1	-1	1
Γ_5	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$

Let us note that the construction of the irreps for a given group G is not a simple mathematical problem. However, the explicit form of all the irreps of point and space groups can be found in many textbooks (see, for example, [Kovalev, 1993]).

The importance of irreducible representations of symmetry groups is illustrated by a famous theorem due to Wigner, according to which eigenstates of any quantum system are classified by irreps of the symmetry group G of its Hamiltonian. Namely, every energy level of the quantum system is associated with a certain irrep Γ_j of the group G , and the *degeneracy* of this level is determined by the *dimension* n_j of the irrep Γ_j .

The normal modes, representing exact vibrational regimes in the harmonic approximation, can be classified in the same manner. Indeed, every eigenstate of the force constant matrix \mathcal{K} (see Eq. (51)) represented by the natural frequency ω_j and the corresponding eigenvector \vec{c}_j can be associated with a certain irrep Γ_j of the parent symmetry group of the considered mechanical system. In both cases, the differential equations describing the physical systems (quantum or classical) are *linear*. In this regard, it is interesting to investigate any possible symmetry – determined classification of exact dynamical regimes in *nonlinear* classical systems with certain parent symmetry groups. This problem is fundamental in the theory of bushes of nonlinear normal modes, as we demonstrate below.

5.4. Selection rules for excitation transfer between modes of different symmetry

Let us return to the discussion of N -degree-of-freedom mechanical systems with the parent symmetry group G_0 whose vibrational state is described by the N -dimensional configurational vector $\vec{X}(t)$.

As has already been discussed, all the vibrational states can be classified by the subgroups of the parent group G_0 . Let us consider the vibrational state characterized by a certain subgroup $G \subset G_0$. This means that the configuration vector $\vec{X}(t)$ must be *invariant* under the action of all the operators $\hat{g} \in \hat{G}$:

$$\hat{g}\vec{X}(t) = \vec{X}(t), \quad \forall \hat{g} \in \hat{G}. \quad (\text{A.18})$$

The group $\hat{G} = \{ \hat{g} \mid \forall g \in G \}$ consists of all the operators \hat{g} which are associated with the elements g of the symmetry group G .

Let us now decompose the configuration space into the minimal subspaces, which are invariant with respect to the parent group G_0 . Every one of these subspaces V_j is the carrier space of a certain irrep Γ_j of the group G_0 . As a result of this transformation, the mechanical representation Γ turns out to be decomposed into a number of irreps:

$$\Gamma = \sum_j^{\oplus} \Gamma_j. \quad (\text{A.19})$$

The set of all the basis vectors $\vec{\varphi}_j^{(i)}$ of the irreps Γ_j entering in the direct sum (A.19) may be chosen as a new basis of the configuration space. Therefore, we can decompose the configuration vector $\vec{X}(t)$ in the

above mentioned basis as follows:

$$\vec{X}(t) = \sum_{ji} \mu_j^{(i)}(t) \vec{\varphi}_j^{(i)} = (\vec{\mu}_j(t), \vec{\Phi}_j) = \sum_j \vec{\Delta}_j(t), \quad (\text{A.20})$$

where $\vec{\Delta}_j(t)$ is the contribution to $\vec{X}(t)$ from the irrep Γ_j , while i indicates different basis vectors of the n_j -dimensional irreducible representation Γ_j . Here we introduce the “supervector” $\vec{\Phi}_j = \{\vec{\varphi}_j^{(1)}, \vec{\varphi}_j^{(2)}, \dots, \vec{\varphi}_j^{(n_j)}\}$ which determines the set of the basis vectors of the irrep Γ_j , the vector $\vec{\mu}_j(t) = \{\mu_j^{(1)}(t), \mu_j^{(2)}(t), \dots, \mu_j^{(n_j)}(t)\}$, which determines the time-dependence of the individual vibrational modes, and their *formal scalar product* $(\vec{\mu}_j(t), \vec{\Phi}_j)$. From the condition of invariance of the configuration vector $\vec{X}(t)$ with respect to the group \hat{G} , (A.18), it can be deduced (see [Sakhnenko & Chechin, 1993; Chechin *et al.*, 2007]) that the following invariance conditions also hold regarding the individual irreps Γ_j :

$$(\Gamma_j \downarrow G) \vec{\mu}_j = \vec{\mu}_j. \quad (\text{A.21})$$

Here we have introduced the *restriction* $(\Gamma_j \downarrow G)$ of the irrep Γ_j of the parent group G_0 onto the subgroup $G \subset G_0$. The restriction $(\Gamma_0 \downarrow G)$ is the set of all the matrices of the representation Γ_0 of the group G_0 which are associated only with the elements of its subgroup $G \subset G_0$.

Eq. (A.21) provides the important *selection rules for excitation transfer* between modes of different symmetry. Let us consider this point in more detail. This equation indeed holds for every individual irrep Γ_j of the parent group G_0 . Thus, from (A.21), we can see that $\vec{\mu}_j$ is *invariant* under all matrices $\mathcal{M}_j(g) \in (\Gamma_j \downarrow G)$, i.e. $\vec{\mu}_j$ is the *common eigenvector* of all the matrices $\mathcal{M}_j(g)$, $g \in G$ with *unit* eigenvalue.

As the general solution of Eq. (A.21), the vector $\vec{\mu}_j$ depends on a number of arbitrary constants denoted by the letters a, b, c, d , etc., in the examples of section III. To find all modes contributing to a given dynamical regime with symmetry group G , expressed in Eq. (A.20) by the vector $\vec{X}(t)$, one must solve the linear algebraic equations (A.21) for each irrep Γ_j of the group G_0 . As a result, the invariant vectors $\vec{\mu}_j$ for some irreps Γ_j may turn out to be equal to zero and thus *not contribute* to the considered dynamical regime. On the other hand, some nonzero invariant vectors $\vec{\mu}_j$ for multidimensional irreps can be very special due to certain relations between their components (for example, some components are equal to each other, or differ only by sign). Naturally, the contributions $\vec{\Delta}_j(t)$ to $\vec{X}(t)$ from such irreps Γ_j also possess very special features.

Actually, Eq. (A.21) can be considered as a source of certain *selection rules* for excitation transfer from the “root” mode to a number of other (secondary) modes. Indeed, if a certain mode with the symmetry group G is excited initially (called the “root” mode), this group determines the symmetry of the whole bush. The condition that the appropriate dynamical regime $\vec{X}(t)$ must be invariant under the action of the above group G leads to Eq. (A.18) and then to Eq. (A.21). If the vector $\vec{\mu}_j$ for a given irrep Γ_j is the zero vector, there are no modes, belonging to this irrep, which contribute to $\vec{X}(t)$, i.e., the initial excitation *cannot be transferred* from the root mode to the secondary modes associated with the irrep Γ_j .

Note that basis vectors associated with a given irrep Γ_j in Eq. (A.20) turn out to be equal to zero when this irrep is not contained in the decomposition of the full natural irrep Γ into its irreducible parts Γ_j . This gives rise to *additional selection rules* which reduce the number of possible vibrational modes in the considered bush. Trying every irrep Γ_j in Eq. (A.21) and analyzing the above mentioned decomposition of the natural representation Γ , we obtain explicitly the whole bush of modes with the symmetry group G .

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